Process Safety and Environmental Protection

Rok 2021, Volume 147

March

Mattia Carboni, Gianmaria Pio, Chiara Vianello, Ernesto Salzano. *Safety distances for the sour biogas in digestion plants*. Pages 1-7.

The presence of sulfur-based substances in the biogas (sour) produced from the digestion plant imposes several treatments to match the market and regulation requirements. Besides, it lays the production plants open to safety and environmental risks related to the accidental release of toxic species. This work is devoted to the investigation of the consequences of the accidental release of biogas containing hydrogen sulfide up to 10 %vol. To this aim, a schematic 3-D representation of a biogas productive plant was developed and implemented in a Computational Fluid Dynamics (CFD) model. The effects of the initial composition and the wind velocity on the cloud dispersion were evaluated. The calculated stand-off distances for lethality resulted from the numerical simulation were compared with the results of standard integral models commonly adopted in the process industry. Results indicated the dramatic effects of the toxicity of hydrogen sulfide on the downwind safety distance in the case of accidental release of sour biogas, and the negligible effects for the flammability concerns.

- **Keywords:** Biogas; Hydrogen sulfide; Computational fluid dynamic; Anaerobic digestor plant

Hanieh Najafi, Samira Farajfaed, Sheida Zolgharnian, Seyed Heydar Mosavi Mirak, Neda Asasian-Kolur, Seyedmehdi Sharifian. *A comprehensive study on modified-pillared clays as an adsorbent in wastewater treatment processes*. Pages 8-36.

Pillared clays are special kinds of modified clays with significant and permanent porosity, produced by embedding columns or pillars between the layers of clay. However, these materials are very well-known for their catalytic properties; their adsorptive characteristics in wastewaters towards different classic and growing contaminants need to be studied comprehensively. The present work is performed to introduce different methods for clays' pillaring, the main steps of the process, comparison of various pillaring agents, etc. During recent years, several investigations have been carried out to find a way for pillared clays' modification (by introducing active chemical functional groups, doping, heat treatment, etc.) to achieve selective adsorbents towards specific pollutants. Therefore, the main modification techniques including surfactant modification, metal doping, etc. are introduced and classified in the present work. Furthermore, adsorptive applications of (modified) pillared clays towards organic, pharmaceutical, and metal ions pollutants, the relationship between physicochemical properties and

adsorption performance of pillared clays, adsorption mechanisms, and quantitative comparison of pillared clays' ability for pollutants removal are the other issues that have been considered in the present work.

- **Keywords:** Pillared clay; Modification; Adsorption; Wastewater; Heavy metals; Pharmaceutical pollutants

Jiqin Wang, Zhouman Huang, Deze Yang, Xiangfei Zeng, Mengjun Chen, Jiancheng Shu, Zhi Sun, Shuhui Sun, Zhengxue Xiao. *A semi-scaled experiment for metals separating and recovering from waste printed circuit boards by slurry electrolysis*. Pages 37-44.

Waste printed circuit boards (WPCBs) are considered as the most complicated and valuable component among e-waste. Slurry electrolysis can separate and recover metals from the extremely complex WPCBs. To promote its industrial application, a 5000mL scale experiment was conducted to confirm industrial feasibility. Those results showed that copper and total metal recovery rates were 94.5 % and 75.2 % under the optimized conditions (30g/L WPCBs, 10g/L CuSO4·5H2O, 30g/L NaCl, 190g/L H2SO4, 30g/L H2O2, 298K temperature, 250r/min stirring speed, 300 A/m2 and 8h). The copper purity was 92.9 %, and SEM-EDS analyses indicated the main dendritic metals recovered were copper and lead. USEtox toxicity potential evaluation results demonstrated human toxicity and ecotoxicity of WPCBs sharply decreased after treatment. A cost analysis of this process indicated that the $ 1.0 cost was partially offset by the $ 1.9 return from 1kg WPCBs. Thus, slurry electrolysis has a promising industrial future for e-waste recycling/utilization.

- **Keywords:** WPCBs; Metals; Separation; Recovery; Slurry electrolysis; Semi-scaled

Xiangyu Shao, Liang Pu, Xin Tang, Shenyin Yang, Gang Lei, Yanzhong Li. *Experimental study of transient liquid nitrogen jet impingement boiling on concrete surface using inverse conduction problem algorithm*. Pages 45-54.

There is a shortage of research in the literature on the evaporation rate of the liquid pool under instantaneous conditions, which is important for the risk assessment of the liquid hazard leakage accidents. Previous perfect thermal contact model and typical pool boiling could not completely represent the boiling process in the spreading liquid pool. In this work, the spreading liquid pool was characterized as a free-surface jet impingement on the plate surface. Liquid nitrogen (LN2) was adopted to simulate liquid hydrogen (LH2) and liquid natural gas (LNG) leakage, and a series of transient jet impingement boiling experiments were conducted on the concrete surface. Liquid jetted upon the stagnation region, and the transient heat flux from the concrete surface was estimated by transfer function method. The boiling curve obtained in the present study appears significantly different from the typical pool boiling, which indicate that large deviation will occur when the typical pool boiling correlations are used for instantaneous leakage, at least for the stagnation region. A point between the onset of nucleate boiling point and fully developed nucleate boiling point was recognized, which represents the turn of forced convection dominated to nucleate boiling dominated. It is confirmed that the heat transfer was enhanced with increased jet height z, and the peak values were found at z/d = 8.

- **Keywords:** Liquid hazards; Instantaneous leakage; Liquid pool; Evaporation rate; Jet impingement boiling

Hans-Peter Schildberg, Julia Eble. *Experimental determination of the static equivalent pressures of detonative explosions of cyclohexane/O2/N2-mixtures in long and short pipes*. Pages 55-67.

In the past 5 years the Safety Engineering Group of BASF has determined the static equivalent pressures ("pstat") of the eight detonative pressure scenarios which explosive gas mixtures can exhibit in long and in short pipes. More precisely, for different combustibles the pstat-values of the corresponding ternary mixtures combustible/O2/N2 were determined on the stoichiometric line and on the O2-line of the explosion triangle. By doing so, the pstat-values of all other compositions inside the explosion triangle could be predicted by extrapolation with an accuracy sufficient for practical applications. Furthermore, a proposal of how to transfer these results to the huge number of other combustibles not investigated so far was provided. A key-parameter in this context was the ratio R between the static equivalent pressure at the point where the deflagration-to-detonation transition occurs in the long pipe and the static equivalent pressure in the region of the stable detonation. In the present work the pstat-values of the new ternary mixture cyclohexane/O2/N2 are reported. Cyclohexane is of special interest because its autoignition temperature (AIT) in air is substantially lower than the AIT-values of all combustibles that have been tested before. According to our hitherto understanding the low AIT should noticeably reduce the ratio R. The experiments, however, did not confirm this hypothesis. After presenting the experimental results, which actually confirm the findings for the combustibles investigated so far, an explanation for the unexpected behaviour regarding R will be presented in terms of the differences between the low-temperature and the high temperature oxidation mechanism. As kind of spin-off, this explanation also allows to better understand quantitatively the degree of precompression in the yet unreacted mixture required for the occurrence of the deflagration-to-detonation Transition (DDT).

- **Keywords:** Low temperature oxidation mechanism; Detonation; Deflagration-to-detonation transition; High temperature oxidation mechanism; Static equivalent pressure; Ignition delay time

Wenjiao Sang, Dong Li, Yongjian He, Cheng Zhan, Qian Zhang, Cuihua Li, Rajendra Prasad Singh. *Sludge reduction and pollutants removal in anaerobic-anoxic-oxic reactor with 2450 MHz electromagnetic wave loading on returned sludge: Performance and mechanism*. Pages 68-79.

To comprehensively evaluate the impact of 2450 MHz electromagnetic wave (EW) loading on returned sludge (RS) for sludge reduction and pollutants removal in anaerobic/anoxic/oxic (A2O) process, the performance of the coupled process (EWRS-A2O) was investigated in current study. 250 W was the appropriate loading power when considering both biological effect and dissolution effect of electromagnetic wave on the returned sludge. After being loaded, floc structure of the returned sludge became looser, and the microbial composition changed. The continuous operation indicated that an 8.3 % improvement in total nitrogen removal and a 33.1 % of sludge reduction were achieved in EWRS-A2O, accompanied by an observed yield coefficient of 0.35 kg SS/kg COD. Although an increase in the total phosphorus concentration of the effluent was found, the impacts on the chemical oxygen demand and ammonia nitrogen of the effluent were minimal. When contrasted to conventional A2O, EWRS-A2O process exhibited higher microbial metabolic activity. Miseq sequencing results showed that the microbial richness increased in EWRS-A2O system with changing of the microbial community structure. Additionally, functional microorganism analysis revealed the enrichment of slow-growing bacteria (Dechloromonas), fermenting bacteria (Clostridium sensu stricto and Tolumonas), and heterotrophic denitrifying bacteria (Thermomonas).

- **Keywords:** Sludge reduction; Anaerobic-anoxic-oxic; Electromagnetic wave loading; Returned sludge; Microbial community

Hans J. Pasman, Bruno Fabiano. *The Delft 1974 and 2019 European Loss Prevention Symposia: Highlights and an impression of process safety evolutionary changes from the 1st to the 16th LPS*. Pages 80-91.

The first European Loss Prevention Symposium under the auspices of the European Federation of Chemical Engineering (EFCE) took place in 1974 in the then new Aula of the Delft University of Technology in the Netherlands. After the triennial symposium over a period of 45 years having been organized in several European cities, it returned in 2019 to the Delft Aula. Authors of this paper are members of EFCE Loss Prevention Working Party organizing the LP Symposia and after nearly half century, it is therefore worthwhile to look back and also to look forward, following the evolution of process safety. This paper presents an impression of the changes in process safety, risk management approaches, and methods over that 45-year period, while at the same time the last symposium contributions are briefly reviewed and a few highlights, called breakthroughs, are identified.

- **Keywords:** Loss prevention; Process safety; Safety topics; Working party on loss prevention

Jianwei Cheng, Xinrui Zheng, Yadong Lei, Wang Luo, Yu Wang, Marek Borowski, Xiaochuan Li, Wanting Song, Zui Wang, Kai Wang. *A compound binder of coal dust wetting and suppression for coal pile*. Pages 92-102.

Increasing expansion of China's coal mine production leads to the increased storage pressure in current coal silos. Most of these coals are stored in open-air coal pile. Therefore, those coal piles have caused a series of environmental pollution problems, which includes endangering workers' health and aggravating air pollution in the surrounding natural environment. Therefore, it is urgent to study and prevent the dust flying problem of coal pile. This paper, based on a single chemical dust suppressant, optimizes a new type of composite binder. This composite binder has advantages of dust suppression effect, relatively simple preparation process and the environmentally friendly agent. This paper is mainly divided into two parts: the study on the influencing factors of dust wetting and the development and application of related spraying systems. Through the energy spectrum analysis of scanning electron microscope and reverse osmosis method, it explores the dust wetting and suppression characteristics of the composite binder with different physical and chemical properties. The optimal application range of the composite binder are obtained. Finally, an automatic spraying system for dust suppression is designed. The composite binder developed in this paper is applied in the open-air coal yard and the results show that the composite binder studied in this paper has a good effect of dust suppression.

- **Keywords:** Coal pile; Composite binder; Reverse permeation; Dust suppression

Wan Ying So, Mimi H. Hassim, Syaza I. Ahmad, Roslina Rashid. *Inherent occupational health assessment index for research and development stage of process design*. Pages 103-114.

Occupational health analyses the job and health relationships, in particular the chronic health influence of chemicals to workers. In most of the previous works for inherent hazards assessment, the focus was put on safety aspect; with very minor elements of health are taken into account. Most of the earlier design stage assessment methods focus only on the hazard identification and assessment part; but not the risk mitigation

element. This study aims to create an assessment method that integrate the existing inherent hazards assessment index which is the Inherent Occupational Health Index (IOHI) with suitable Layers of Protection (LOP) strategies for each of the enlisted hazard parameters. The IOHI considers the health hazards existed during research and development stage. Risk prevention and minimization strategies are proposed according to each hazard parameters and levels. Scores are also assigned to each LOP strategies. Integration of occupational health hazard assessment index with the prevention strategy is achieved through a designed formula. The proposed method provides users with list of suitable counter measures for each hazard parameter, and each option offers varied level of effectiveness. The proposed index is applied to two process routes of methyl methacrylate production which are ethylene via propionaldehyde based route (C2/PA) and propylene based route (C3). The results revealed that the process routes are in the category of "safe" when the proposed control strategies are evaluated in the assessment.

- **Keywords:** Inherent health; Index development; Risk prevention; Minimization strategies; Research and development; Design stage

Leonardo Leoni, Ahmad BahooToroody, Mohammad Mahdi Abaei, Filippo De Carlo, Nicola Paltrinieri, Fabio Sgarbossa. *On hierarchical bayesian based predictive maintenance of autonomous natural gas regulating operations*. Pages 115-124.

Safety Improvement of engineering processes, especially Oil & Gas operations, has gained a lot of attention during the last decades. This fundamental vision results in risk remediation programs, minimizing the risks of failure, and reducing the associated costs for operation and maintenance. As failures may represent serious threats for both humans and the environment, a comprehensive tool is required to employ maintenance and avoid immoderate dangerous consequences. Traditional risk frameworks mainly include estimation approaches, such as Fault Tree (FT) and Event Tree (ET), producing more simplified models than other tools, such as Bayesian inference. The present work aimed at developing an advanced Risk-Based Maintenance (RBM) methodology for prioritizing maintenance operations, by addressing associated uncertainties through the accident modelling of the process. For this purpose, a Hierarchical Bayesian Approach (HBA) is applied to estimate the failure probabilities of each component while a Failure Mode, Effects and Criticality Analysis is performed to assess the severity. With Markov Chain Monte Carlo simulation from likelihood function and prior distribution, the HBA is capable of incorporating the fluctuations and uncertainties associated with operational data including the variability between the source of data and the correlation of observations. Lastly, to make a meaningful difference between different kinds of risk consequences, whether the risk has a direct or indirect loss, the cost of failures of components is accounted for. To demonstrate the application of the methodology, a Natural Gas Reduction and Measuring Station (NGRMS) is taken into account as a case study. The outcome of the case study proofed that PTG and pump are the most failures sensitive components among other if they being left unattended in the operation with an average number of failure occurrences of 67 and 45; While the THT pipelines and THT tank are less sensitive for being considered for major maintenance request with almost average of 5 times in their lifetime. The proposed method can be exploited by maintenance engineers, asset managers, and policymakers to reduce the downtime periods as well as the risks of on-going operations.

- **Keywords:** Risk-based maintenance; Markov Chain Monte Carlo simulation; Hierarchical Bayesian approach; Autonomous operation

Taiyu Luo, Jie Yang, Yunhao Li, Yuan Yu, Yifan Suo, TingTing Chen, Ning Song, Changxin Li, Juncheng Jiang. *The effects of thermal pyrolysis and*

***decomposition products on explosive characteristics of flufenacet and sulfentrazone*. Pages 125-133.**

Thermal pyrolysis and decomposition products of flufenacet and sulfentrazone powders were tested by thermogravimetric analysis (TGA), TGA coupled with Fourier transform infrared spectroscopy and pyrolysis-gas chromatography/mass spectrometry. Besides, the explosion sensitivity (minimum ignition temperature, minimum ignition energy, minimum explosion concentration) and explosion severity (maximum explosion pressure, and the maximum rate of pressure rise) were measured in standard 20-L spherical chamber, Hartmann apparatus and Godbert-Greenwald Furnace apparatus. Moreover, the effect of thermal pyrolysis characteristics on the explosion sensitivity and severity of flufenacet and sulfentrazone dust clouds were analyzed. The results indicated that flufenacet had lower decompose temperature, and smaller activation energy than sulfentrazone. Both flufenacet and sulfentrazone expressed flammable and toxic substance during their decomposition. Greater amount of products with higher flammability were expressed from flufenacet compared with sulfentrazone. The flufenacet had lower explosion sensitivity than sulfentrazone In addition, the flufenacet's explosion severity was higher than sulfentrazone, which was mainly determined by the larger number of combustible gases from flufenacet. What's more, both the two herbicide powders can lead to serious dust explosion accidents due to their explosive and toxic characteristics.

- **Keywords:** Thermal pyrolysis; Flufenacet powder; Sulfentrazone powder; Explosion sensitivity; Explosion severity

Ting Sun, Xiangning Liu, Xiaozhen Zhan, Lingling Ou, Renfa Lai. *Hepatic distribution and toxicity of zirconia nanoparticles in vivo and in vitro*. Pages 134-145.

Zirconia nanoparticles (ZrO2-NPs) have been increasingly used in industrial, biomedical and dental materials. Nevertheless, the scientific basis for the toxicological effects of ZrO2-NPs is poorly elucidated, and the understanding of the underlying mechanism is still limited. The hepatic biodistribution and toxicological effects of ZrO2-NPs after a single intravenous administration (20 mg/kg bw) in vivo and the toxicological mechanism toward hepatocytes in vitro were investigated. The liver showed continuous ZrO2-NP accumulation over a 28-d period. Moreover, ZrO2-NPs induced steatosis, functional injury, inflammatory response, and gene alternations in the liver. The main gene altered pathways induced by ZrO2-NP exposure were involved in metabolism, cellular processes, and human diseases. Among these pathways, lipid biosynthesis and metabolism alterations were predominant, and P53 signaling was also identified. Precious gene expression quantification further showed alterations in genes related to lipid biosynthesis and metabolism and cell apoptosis. Meanwhile, the results of the in vitro studies demonstrated ZrO2-NPs induce oxidative stress, lipid accumulation, cell apoptosis and P53-mediated signaling pathway activation in HepG2 cells. This study proves that ZrO2-NPs have impacts on the liver. There is potential concern over the hepatotoxicity of ZrO2-NPs in biomedical applications and occupational exposure through large-scale production.

- **Keywords:** Zirconia nanoparticles; Hepar; Distribution; Toxicity

Kai Wang, Weiyao Cai, Yuchen Zhang, Haiqing Hao, Ziting Wang. *Numerical simulation of fire smoke control methods in subway stations and collaborative control system for emergency rescue*. Pages 146-161.

As subway fires can easily cause numerous casualties, this paper proposes the idea of active disaster relief, which involves ventilation, exhaust, smoke blocking and exhaust,

and other facilities coordinating centralised control to assist passenger evacuation and firefighting. The ventilation and smoke exhaust method used in multilayer crossing complex subways is analysed, and a typical interchange transfer station is selected to build a numerical model. The combined control of fire smoke is analysed based on six ventilation modes, and fire dynamics simulator software is used to perform several numerical simulations. According to the simulation results, ventilation and smoke control is used in the cases of fire on the second and third floor in the underground, the airflow speed of the stairway reached 2 m/s, which can completely restrain the smoke on the fire floor. According to the characteristics of different fire sources and smoke control scenarios, a remote monitoring model of multielement information fusion, such as ventilation path, fan characteristics, smoke exhaust channel, and smoke blocking facilities, is established, and a multielement disaster information-fusion-based collaborative centralised emergency rescue platform for subway fire disaster relief is developed. Real-time disaster analysis is performed, and intelligent control of airflow and smoke exhaust in the complex form of subway-controlled smoke turbulence field is developed to facilitate safe escape and efficient firefighting and rescue of people during emergencies.

- **Keywords:** Subway fire; Smoke isolation; Mechanical smoke extraction; Information fusion; Collaborative centralised control

Arvind Kumar, Basheswar Prasad, Krishan Kishor Garg. *Enhanced catalytic activity of series LaCuxFe1-xO3 (x = 0.2, 0.4, 0.6, 0.8) perovskite-like catalyst for the treatment of highly toxic ABS resin wastewater: Phytotoxicity study, parameter optimization and reaction pathways*. Pages 162-180.

In the present study, acrylonitrile butadiene styrene (ABS) resin wastewater was treated by series LaCuxFe1-xO3 (x = 0.2, 0.4, 0.6, 0.8) perovskite-like catalyst activated with peroxymonosulfate (PMS). The catalyst was synthesized by solgel method and further characterized by various techniques including i.e., XRD, FTIR, BET, FE-SEM with EDAX, TEM and XPS. Phytotoxicity study was performed to assess the toxicity of ABS resin wastewater on common agriculture crops viz., Vigna radiatus L. (Mung) and Hordeum vulgare L.(Barley). The effect of various parameters e.g., catalyst dosage (250−1050 mg/L), PMS dosage (1−5 mM), pH (2−10) and temperature (30−90 °C) were evaluated and optimize the parameters through central composite design (CCD) in response surface methodology (RSM). The maximum removal of acrylonitrile and TOC were observed 94.06 % and 66.70 %, respectively at optimum operating conditions obtained from RSM tools. The kinetic studies for the degradation of acrylonitrile and TOC was performed by two step pseudo first order kinetic model at various temperatures (30−90 °C). Catalyst reusability and chemical stability study were analyzed and degradation of acrylonitrile i.e., 94.06 %, 91.38 %, 88.42 % and 86.92 %; and TOC i.e., 66.70 %, 64.35 %, 61.59 % and 59.21 % were observed in first, second, third and fourth consecutive cycles. The proposed reaction pathways and PMS activation mechanism were investigated based on intermediate detected from GC–MS analysis and scavenger experimental study. Operating cost of treatment of ABS resin wastewater was estimated to be 75.60$/m3 wastewater.

- **Keywords:** Acrylonitrile; Peroxymonosulfate; Perovskite; Optimization; Degradation

Katarzyna Glińska, Jaume Gitalt, Esther Torrens, Natalia Plechkova, Christophe Bengoa. *Extraction of cellulose from corn stover using designed ionic liquids with improved reusing capabilities*. Pages 181-191.

In recent years, the dissolution of lignocellulosic biomass using ionic liquids has attracted a lot of attention. Generally, the processes of valorisation of residual biomass do not extract cellulose. Among the lignocellulosic biomass, corn stover has a great interest because its high content in cellulose. For this reason, five ionic liquids have been designed and produced to dissolve the cellulose contained in corn stover, three tetra-alkyl-phosphonium based ILs and two imidazolium based ILs: tetra-butyl-phosphonium acetate [P4444][OAc]; tri-butyl-methyl-phosphonium acetate [P4441][OAc]; tetra-butyl-phosphonium 2-ethyl-hexanoate [P4444][EH]; 1-dodecyl-3-methyl-imidazolium bis (2,4,4-tri-methyl-pentyl) phosphinate [C12mim][(iC8)2PO2]; 1-decyl-3-methyl-imidazolium bis (2,4,4-tri-methyl-pentyl) phosphinate [C10mim][(iC8)2PO2]. The dissolution of cellulose was carried out under mild conditions (3 h and 80℃). Among the synthesised ionic liquids [P4444][EH] turned out to dissolve the greatest amount of cellulose (84 %), while imidazolium ionic liquids [C12mim][(iC8)2PO2] and [C10mim][(iC8)2PO2] dissolved 61.1 % and 44.0 %, respectively. On the other hand, these designed ILs have the ability to be easily recovered. As they are microemulsion-forming ionic liquids, the recycling of these ionic liquids was more straightforward (without the need of solvent evaporation). Furthermore, imidazolium ionic liquids were found to eliminate more ashes from the corn stover than tetra-alkyl-phosphonium ionic liquids.

- **Keywords:** Corn stover; Cellulose extraction; Ionic liquids; Hydrophilic tetra-alkyl-phosphonium ionic liquids; Microemulsion-forming imidazolium ionic liquids

Sahar Foorginezhad, Masoud Mohseni-Dargah, Khadijeh Firoozirad, Vahid Aryai, Amir Razmjou, Rouzbeh Abbassi, Vikram Garaniya, Amin Beheshti, Mohsen Asadnia. *Recent Advances in Sensing and Assessment of Corrosion in Sewage Pipelines*. Pages 192-213.

Corrosion is known as the gradual destruction of materials, leading to structural integrity loss and deteriorates the surface function. Regarding sewage pipelines, corrosion is vital due to its substantial financial, health, and safety costs for society, and it is considered as one of the biggest problems facing water and wastewater infrastructure. Also, it is the primary cause of chemical property alteration, efficiency loss, life span reduction, etc. To overcome the resulting problems, various researches have been performed to understand not only the effective parameters leading to corrosion in sewer pipes but also monitoring the infrastructure conditions. Studies have depicted that developments in sensing systems to detect effective parameters in pipe corrosion such as temperature, H2S, and pH, have significantly reduced damage to the industrial equipment of sewage pipelines caused by corrosion. This paper presents a critical review of the effective factors resulting in sewer pipeline corrosion and discusses advanced sensing systems utilized for relevant monitoring. Also, microbiologically induced corrosion and effective factors are individually discussed. Moreover, various data analysis techniques adopted to evaluate outputs of the sensors for corrosion prediction have been explored. Finally, recommendations and future directions for improving sensing accuracy and robustness are detailed.

- **Keywords:** Corrosion sensor; Structural health monitoring; Humidity sensor; pH sensor; Sewer pipelines; H2S detection; Data processing

Priyanka Sarkar, Apurba Dey. *Phycoremediation: an emerging technique for dye abatement: an overview*. Pages 214-225.

Treatment of dye-containing wastewater is a major challenge for mankind that has gained much interest from the scientific community owing to the growing concerns of environmental safety and legislations. Thus, it becomes imperative to explore green and self-sustainable dye abatement methods. Phycoremediation is emerging as a new age technology with the goal of decolorization and detoxification of the hazardous dye laden effluents. The underlying mechanisms of phycoremediation of dyes are biodegradation,

biosorption, and biocoagulation, which are influenced by several physicochemical and biological factors such as pH, temperature, contact time, surface characteristics, concentration and particle size of the algal biomass, chemical composition and concentration of the dye. This review provides a comprehensive insight into the potential, performance, and applications of phycoremediation methods in terms of the mechanisms, major determinants of phycoremediation processes, physical and chemical pretreatment methods of the algal biomass, and their effects on dye removal. The present article also discusses the emerging aspects of phycoremediation such as immobilization of algae, algal nanoparticles, activated carbon, and algal microbial fuel cell (A-MFC) for dye remediation along with the research gaps and future prospects. It was concluded from the literature review that immobilized algae and algal biochar exhibit enhanced dye uptake capacity due to improved porosity and surface characteristics. A-MFC can be used for simultaneous wastewater treatment and electricity generation. Furthermore, the generation of value-added products from algal biomass used in wastewater treatment has the potential for waste to wealth creation resulting in the improvement in economic feasibilities of the treatment process.

- **Keywords:** Algae; Algal nanoparticles; Algal-MFC; Biodegradation; Biosorption; Decolorization

Sanjay Pindar, Nikhil Dhawan. *Rapid recycling of spent lithium-ion batteries using microwave route*. Pages 226-233.

The discarded lithium-ion batteries containing valuable metals and graphite are excellent resources in the context of urban mining. In the present study, electrode sheets of mixed spent lithium-ion batteries were crushed, sieved, followed by froth flotation for physical separation of graphite values. The current study investigates the carbothermal reduction of the active cathode material in a microwave furnace under ambient conditions using recovered graphite. The microwave response of "as such" active material (mixed anode and cathode), and "separated" active cathode material at 800W, 2.5GHz, was compared. The magnetic product at the optimum condition (850°C, 30 % C, 10min) consists of 73 % Co, 13 % Mn, 6 % Ni, 8 % O and saturation magnetization of 108emu/g, and lithium extraction rate: 93 %. Higher recovery of metal and graphite values are obtained by processing of "separated" cathode material compared to "as such" active materials. The effect of microwave treatment was found successful for metal dissolution in the hydrometallurgical route also. The average activation energy is 72 and 94kJ/mol for "separated" and "as such" active materials, respectively. The cost calculations show that the process is economical.

- **Keywords:** Microwave; Reduction; Recycling; Lithium-ion batteries; Lithium; Cobalt

Gaoming Wei, Hu Wen, Jun Deng, Zhenbao Li, Shixing Fan, Changkui Lei, Mingyang Liu, Lifeng Ren. *Enhanced coalbed permeability and methane recovery via hydraulic slotting combined with liquid CO2 injection*. Pages 234-244.

Enhanced and efficient recovery of coalbed methane (CBM) is essential to prevent mine disasters and utilize unconventional gas resources. In this study, hydraulic slotting (HS) combined with liquid CO2 (LCO2) injection was employed to enhance coalbed permeability and the efficiency of methane recovery from a high-gas and low-permeability coalbed. First, mercury intrusion porosimetry and scanning electron microscopy experiments were conducted to analyze the variations in the coal microstructure and the permeability after HS combined and LCO2 freezing–thawing was conducted under laboratory conditions. The results indicated that the basic parameters of pore structures increased significantly for the treated coal; for instance, porosity and permeability increased by 47.65 % and 65.31 %, respectively. This indicated that coal

permeability increased significantly under multiple stresses induced via HS and LCO2 freezing–thawing. Subsequently, a simulated experiment of LCO2 injection to enhance CH4 recovery from coal was performed; the results thus obtained revealed that LCO2 injection into a high-gas-content coalbed can enhance CBM recovery with an average efficiency of >90 %. Furthermore, an in-situ test indicated that the effective radii for HS and LCO2 injection were 2.5m and 10m, respectively. The results of a 90-d-long methane extraction revealed that the efficiency of CBM recovery increased by a factor of >2.2 and that the residual gas content in the test coalbed was <8.0m3/t after the use of HS combined with LCO2 injection. Additionally, the time required to meet methane extraction standards was reduced significantly.

- **Keywords:** Hydraulic slotting; Liquid CO2 injection; Coal microstructure; Coalbed permeability; Methane recovery

Rohit Chauhan, Vimal Chandra Srivastava. *Superior reduction of nitrate with simultaneous oxidation of intermediates and enhanced nitrogen gas selectivity via novel electrochemical treatment*. Pages 245-258.

This study reports an electrochemical reduction of the NO3− along with oxidation of the in-situ generated NH4+ with maximum selectivity of the N2 gas as the final-product. The use of aluminum as a cathode and Ti/RuO2 as an anode showed enhanced electrochemical nitrate reduction at the cathode and oxidation of the ammonium ion at the anode. Effects of various parameters like initial NO3− concentration (Co = 100−400 mg L−1), a dose of the Cl− as NaCl (NaCl = 100−400 mg L−1), current density applied (j = 83.3-333.3 A m−2), solution pH (pH = 4–10) and electrolysis time (t = 0−120 min) were studied in terms of NO3− reduction and total nitrogen (TN) removal efficiencies. Current efficiency (CE) was elaborated with respect to end products like N2, NO2− and NH4+. Specific electrical energy consumption (SEC) was calculated in kWh kg−1 NO3− removed for the electrochemical process. Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) were utilized for understanding the oxidation/reduction mechanism over electrodes and the characteristics of the electrodes in a different solution. The studied mechanism suggested a circular conversion of NO3− through complex processes into the N2 gas as the final product. The ultimate nitrate and TN degradation efficiency of ≈95 % with N2 selectivity of ≈100 % were achieved at the optimum condition of Co = 100 mg L−1, NaCl = 300 mg L−1, j = 333.3 A m−2, pH = 6 and time = 120 min with SEC = 927.4 kW h kg−1 NO3− removed. The 1st, 2nd, and nth-order kinetic models were used for the reaction kinetics. FE-SEM, XRD, and AFM techniques were used for the characterization of the electrodes before and after all the electrochemical runs. The operating cost was calculated for lab-scale treatment along with a comparison with previous studies. No sludge or scum got produced for each electrochemical run. Finally, this study delivers a superior perceptive for electrochemical characteristics of Al at the cathode side and Ti/RuO2 at anode side as well as electrochemical NO3− reduction and oxidation of the generated NH4+, simultaneously.

- **Keywords:** Nitrate reduction; NH4+oxidation; N2selectivity; Current efficiency; Kinetics; Cost analysis

Hongbin Liu, Jie Yang, Yuchen Zhang, Chong Yang. *Monitoring of wastewater treatment processes using dynamic concurrent kernel partial least squares*. Pages 274-282.

To meet the standards of effluent quality in wastewater treatment processes (WWTPs), a dynamic concurrent kernel partial least squares (DCKPLS) method is proposed for process monitoring. After integrating the augmented matrices and kernel technique, the proposed method can be used to handle the dynamic and nonlinear characteristics of WWTP data simultaneously. Besides, the inherent limitation of PLS decomposition can be overcome by DCKPLS model, which concurrently partitions the feature space data and

output variables into five subspaces. Monitoring performance is evaluated by simulated sensor faults of industrial WWTP data. Specifically, the fault detection rates of bias fault and drifting fault using DCKPLS are increased by 22.65 % and 8.06 %, respectively, in comparison with CKPLS. It is also shown that the DCKPLS model provides better monitoring performance than the other counterparts.

- **Keywords:** Concurrent kernel partial least squares; Dynamic processes; Fault detection; Quality monitoring; Wastewater treatment processes

Sina Keramati, Milad Ferdowsi, Seyed Morteza Zamir. *Compounds interactions during simultaneous biodegradation of hydrophobic n-hexane and hydrophilic methanol vapors in one- and two-liquid phase conditions*. Pages 283-291.

Simultaneous biodegradation of n-hexane (H) and methanol (M) was studied in batch culture in the concentration range of 5−10 g m−3 and 1−5 g m−3, respectively, in the absence and presence of 5−10 % v/v silicone oil. The addition of oil likely increased the mass transfer of H and ended up to H removal efficiency (REH) improvement from 72 – 86 % to 92–94 %. In contrast, M removal efficiency (REM) decreased from 15-−34 % to 6–24 %, due to an increase in the M partition coefficient from 0.00018 to 0.003. Based on statistical analysis, REH and REM of 90 % and 24 % were obtained at optimum condition of 5 g m−3, 1 g m−3, and 5 % v/v for H, M, and oil fraction, respectively. Kinetic study based on Michaelis- Menten for H biodegradation showed that the presence of 5 % v/v oil could decrease the inhibition effect of the presence of M by increasing Vmax from 123 to 133 mg H (g biomass d)−1 and decreasing Km from 21 to 17 g m−3. Also, degree of mineralization increased from 27–29 % in the absence of oil to 35–43 % in the presence of oil for the identical experiments. According to 16S rDNA sequence analysis, Bacillus cereus and Pandoraea pnomenusa were identified as the main H and M degrading species, respectively, with REs >99 %.

- **Keywords:** Henry’s law constant; Kinetic; Optimization; Mineralization; 16S rDNA

Dong Ma, Botao Qin, Yuan Gao, Jianan Jiang, Baochao Feng. *An experimental study on the methane migration induced by spontaneous combustion of coal in longwall gobs*. Pages 292-299.

Once the methane concentration reaches the explosion limit, it may be ignited by coal fires in methane-rich and coal combustion-prone longwall mining gobs. Therefore, the methane migration in the area of spontaneous combustion of coal is important for evaluating the safety risk and revealing the formation mechanism of methane explosions. A self-designed experimental platform of a longwall gob was applied to investigate the methane migration process induced by the spontaneous combustion of coal. The effect of temperature, and range of coal spontaneous combustion on the methane distribution was studied, and the potential area subject to a methane explosion was identified and calculated quantitatively. Furthermore, the methane movement near the area of spontaneously combusting coal was analyzed, and the mechanism of methane accumulation was proposed. The results illustrate that the changes in the temperature and the range of spontaneous combustion of coal affect the migration of the methane concentration in the gobs.

- **Keywords:** Methane movement; Coal mining; Spontaneous combustion; Explosion

Qiang Li, Dongxu Wang, Mingyu Zhao, Minghao Yang, Jianfeng Tang, Kai Zhou. *Modeling the corrosion rate of carbon steel in carbonated mixtures of MDEA-based solutions using artificial neural network*. Pages 300-310.

Amine-based CO2 absorption process has the benefit of purifying produced natural gas and reducing greenhouse gas emissions; however, it is associated with corrosion issues. This work aims to develop a corrosion prediction model for carbon steel in methyldiethanolamine (MDEA)-based binary mixtures with monoethanolamine (MEA), diethanolamine (DEA), or piperazine (PZ) at various concentrations using artificial neural network (ANN). Experimental studies of Q345R steel are performed, and corrosion rate data obtained by weight loss method is used to create a database for training and testing of the ANN model. A backpropagation (BP) multilayer perceptron (MLP) network with three layers is proposed. The number of input variables for the input layer is optimized after performing a correlation analysis. Effect of neuron quantity in the hidden layer on ANN model performance is studied; increasing the neuron quantity in the hidden layer is found to enhance the training accuracy and reduce the testing accuracy. A new index, max absolute relative deviation (MARD), is introduced to quantify the performance of the ANN model. The developed 5-8-1 type ANN model is able to give a MARD of 8.66 %. The same corrosion rate database is used to develop the SVM model, in which radial basis function (RBF) is used as the kernel function, and K-fold cross-validation technique is applied to select the optimal model values. A comparison of performance in both training and testing shows that the ANN model outperforms the SVM model.

- **Keywords:** Amine solution; Corrosion prediction; ANN; Carbon steel

Nassim Khirouni, Augustin Charvet, Clara Drisket, Alain Ginestet, Dominique Thomas, Denis Bémer. *Precoating for improving the cleaning of filter media clogged with metallic nanoparticles*. Pages 311-319.

Filtration of dust nanoparticles emitted from metallurgical processes is currently problematic, due to a rapid increase of the pressure drop and an inefficient filter cleaning, inducing high maintenance costs. This paper investigates the use of precoating technique to overcome the cleaning difficulties caused by the metallic nanoparticles. It consists of protecting the filter surface with a dust layer composed of micron-sized particles that is easily discharged upon cleaning. In this study, the pulse-jet cleaning of flat filters with and without precoating is evaluated. The aim is to determine the effect of operating conditions on the cleaning efficiency and provide guidelines on the application of precoating. Different precoating materials are tested, to determine whether the material choice is of influence. Experimental results highlighted the increase of the collection efficiency and dust holding capacity using precoating. The cleaning efficiency was significantly improved from 10 % without precoating to 90 % with precoating. Clogging/unclogging cycles showed that the use of precoating allowed stabilizing the filtration process.

- **Keywords:** Filtration; Metallic nanoparticles; Cleaning efficiency; Filter media; Precoating

Jian Sun, Gang Zhou, Cunmin Wang, Rulin Liu, Yanan Miao. *Experimental synthesis and performance comparison analysis of high-efficiency wetting enhancers for coal seam water injection*. Pages 320-333.

To improve the wettability effect of coal seam water injection, and reduce dust production from the source, this paper proposes the preparation of three kinds of high-efficiency wetting enhancers. In this study, 2-acrylamide-2-methylpropionic sulfonic acid and itaconic acid were introduced into the polymer chain of sodium alginate in different combinations. Anionic surfactant sodium dodecyl sulfate and nonionic surfactant aliphatic alcohol polyoxyethylene ether were added in different proportions to obtain three kinds of enhancers. The three kinds of enhancers have good viscosity and fluidity, and the optimal emulsifier additive is determined by a surface tension test. The hydrophilic hydroxyl, carboxyl or sulfonic groups of enhancers were obtained by a Fourier-transform infrared experiment, which was beneficial to water absorption. The contact effect of

different solutions on coal block was studied by a scanning electron microscopy experiment. An energy dispersive spectrometry experiment proved that the solution was well dispersed. Through reverse osmosis experiment and contact angle analysis, the wettability of different solutions was compared, and the best enhancers was obtained. The molecular dynamics simulation was used to verify the relationship between them, and finally the mechanism of action was deduced. It was proved that AMPS-IA/SA+SDS/AEO had better wettability. Thus, AMPS-IA/SA+SDS/AEO is an ideal enhancer for coal seam water injection.

- **Keywords:** Coal seam water injection; Enhancer; Sodium alginate; Wettability; Action mechanism

Jungho Sohn, In Sik Hwang, Jungho Hwang. *Improvement of ammonia mixing in an industrial scale selective catalytic reduction De-NOx system of a coal-fired power plant: A numerical analysis*. Pages 334-345.

In this study, several methods are proposed to improve the denitrification (De-NOx) performance of the selective catalytic reduction (SCR) system. To illustrate how the proposed methods can be applied, the numerical analysis for the SCR system of an industrial-scale thermal power plant is conducted. There are two important indices affecting the performance of SCR system: one is the degree of mixing of the injected NH3 and the other is the uniformity of flow velocity before entering the catalyst layer. To improve the NH3 mixing, a static mixer in a location downstream of the ammonia injection grid (AIG) is generally installed. However, the uniformity of flow velocity distribution is severely aggravated as the mixer induces vortex. Therefore, it is suggested to place the mixer away from the catalyst layer to enhance the NH3 mixing and the uniformity of flow velocity together. The effect of the number of injection nozzles of the AIG on the SCR performance is also investigated. The number of nozzles of the ammonia injection grid can be reduced without affecting the uniformity in flow velocity. However, too much reducing the number of nozzles would result in improper ammonia mixing. Therefore, it is recommended to reduce the number of nozzles within a tolerable range of the NH3 mixing.

- **Keywords:** Selective catalytic reduction; Numerical simulation; Static mixer; Vortex mixing; Coal-fired power plant

Eder Carlos Lopes Coimbra, Ann H. Mounteer, Andreiva Lauren Vital do Carmo, Marc Jaqueline Frank Michielsen, Lucas Alcântara Tótola, Júlia Pires Fujiara Guerino, Júlia Gabriela Alves Nogueira Gonçalves, Priscila Romana da Silva. *Electrocoagulation of kraft pulp bleaching filtrates to improve biotreatability*.Pages 346-355.

Bleached kraft pulp mills generate large volumes of effluents usually treated by biological processes that don´t remove recalcitrant organic constituents. The present study was undertaken to evaluate the potential of electrocoagulation of acid (AcF) and alkaline (AlF) kraft pulp bleaching filtrates with Al and Fe electrodes to improve their biotreatability. Response surface methodology was used to predict the effects of initial pH, current density, and electrolysis time on biodegradability (BOD/COD). Biodegradability increases of 1.7–2.1-fold were obtained using optimized experimental conditions for each electrode-filtrate combination: AcF-Al (pH 7.9, 128 A/m², 49 min), AcF-Fe (pH 4.6, 104 A/m², 40 min), AlF-Al (pH 3.8, 150 A/m², 52 min) and AlF-Fe (pH 6.3, 101 A/m², 42 min). Electrocoagulation with Al electrodes was more efficient in removing color, phenols and estrogenic activity, but required longer reaction time and higher current density, while treatment with Fe electrodes resulted in lower toxicity to Daphnia similis. Electrocoagulation of both filtrates before combining them for biological treatment led to 88 % dissolved organic carbon (DOC) removal in a five-day biodegradability test,

compared to only 27 % DOC removal from combined raw filtrates. The potential to increase overall pulp mill wastewater treatment efficiency using electrocoagulation prior to biological treatment was demonstrated.

- **Keywords:** Biodegradability; Response surface; Toxicity; Wastewater

Esrafil Asgari, Amir Sheikhmohammadi, Heshmatollah Nourmoradi, Shahram Nazari, Mohammad Aghanaghad. *Degradation of ciprofloxacin by photocatalytic ozonation process under irradiation with UVA: Comparative study, performance and mechanism*. Pages 356-366.

The photocatalytic ozonation process (O3/UVA/TiO2) was applied for the removal of ciprofloxacin antibiotic (CIP) from aqueous solutions. The influence of various operational factors such as solution pH, initial pollutant concentration, catalyst content, ozone dose and scavengers was studied on the process. The mineralization, biodegradability, kinetic models, catalyst recyclability, electrical energy consumption and cost estimation of the process were also performed. Various techniques of FE-SEM, EDS, FTIR, XRD and UV–vis were applied to characterize the catalyst. The highest CIP removal (98.5 %) was obtained in ozone and catalyst doses of 0.34 g/h and 1.0 g/L, respectively during 15 min reaction time at pH 9.0. The scavenging experiments approved the contribution of hydroxyl radicals (OH) and superoxide (O2−) as the main active radical species in the process. The competition effect of various anions on the process efficiency was in the order of chloride > carbonate > bicarbonate > sulfate. The process kinetics followed the pseudo-first-order model. The catalyst efficiency was about 95 % of the original one after 6 recycling steps. It can be concluded that the photocatalytic ozonation process (O3/UVA/TiO2), due to the low reaction time and high removal efficiency, can be considered as a suitable and practical technique for the removal of antibiotics from aqueous solutions.

- **Keywords:** Photocatalytic ozonation; Ciprofloxacin; Mineralization; Energy consumption

Augustine Uhunoma Osarogiagbon, Faisal Khan, Ramachandran Venkatesan, Paul Gillard. *Review and analysis of supervised machine learning algorithms for hazardous events in drilling operations*. Pages 367-384.

Results of bibliometric analysis and a detailed review are reported on the use of supervised machine learning to study hazardous drilling events. The bibliometric analysis attempts to answer pertinent questions related to progress in the use of supervised machine learning for hazardous events due to drilling fluid density/mud weight. The analysis indicates artificial neural network as the most popular algorithm among researchers. Also, deep learning, random forest and support vector machine have gained momentum in recent use. A critical review of literature on hazardous events and supervised machine learning algorithms are reported. This review was done to observe how the algorithms were used, their relative successes, limitations, as well as input parameters which aided in detection or estimation by the machine learning algorithms. An introduction to deep learning and a review of literature on the use of deep learning with respect to operations involving drilling parameters is presented. The review on deep learning and drilling parameters covered the following operations: lithology identification, drilling rig state determination, generating logging/other drilling parameters and detecting abnormality in data. The study highlights need of publicly accessible large database with data from different oilfields for development of machine learning algorithms. These algorithms could be used globally for the enhancement of machine learning for new fields or fields with limited data. The availability of such large database

would aid researchers in improving or customizing deep learning algorithms in line with the unique needs of drilling activities.

- **Keywords:** Machine learning; Artificial intelligence; Deep learning; Bibliometric analysis; Drilling operation; Drilling safety; Petroleum industry

Yi-Ju Wu, Yi-Wen Liu, Hai-Hsuan Cheng, Chih-Wen Ke, Tsair-Fuh Lin, Liang-Ming Whang. *Biological pre-treatment system for ammonia removal from slightly contaminated river used as a drinking water source*. Pages 385-391.

A pilot-scale biological pre-treatment reactor filled with porous polyurethanes carriers (BioNET) was operated over 500 days under different hydraulic retention times (HRT) (1.3 to 0.5 h) to evaluate the feasibility and efficiency of ammonia removal for a slightly contaminated source water. Under 0.5 h HRT, 84 % nitrification efficiency and 0.42 kg-N/m3/day ammonia removal rate could be achieved with influent ammonia concentration of 10.4 mg N/L. Results of batch tests indicated that the effect of aeration on nitrification of BioNET was more significant than temperature and components in raw water. Specific ammonia oxidization rate for batches with aeration were 4.5–9.1 times higher than those without aeration. In addition, simultaneous nitrification and denitrification were observed with batch tests using BioNET obtained from the reactor. Ammonia monooxygenase subunit A (amoA) gene of ammonia oxidizing archaea and bacteria (AOA and AOB) and 16S rRNA gene of total bacteria, Nitrospira, and Nitrobacter were quantified using real time quantification polymerase chain reaction (qPCR). AOB and Nitrospira were dominant in the bioreactor. Higher nitrification efficiency (>60 %) could be achieved at AOB abundance higher than 1.25 × 108 copy/BioNET and AOB/TB higher than 1.2. This study demonstrated that the BioNET system can be a promising technology for removing ammonia from slightly polluted river water at a low HRT condition.

- **Keywords:** nitrification; denitrification; BioNET, ammonia; AOB abundance

Hassan Alamgholiloo, Bayram Hashemzadeh, Nader Noroozi Pesyan, Amir Sheikhmohammadi, Esrafil Asgari, Jaber Yeganeh, Hassan Hashemzadeh. *A facile strategy for designing core-shell nanocomposite of ZIF-67/Fe3O4: A novel insight into ciprofloxacin removal from wastewater*. Pages 392-404.

byproducts with low toxicity for enhancing the quality of drinking water and wastewater has remained a huge challenge for environmental aim. In this study, a nanocomposite based on Cobalt zeolite imidazolate framework (ZIF-67), and Fe3O4 nanoparticles (NPs) were prepared using the simple sol-gel method. In this nanocomposite, Fe3O4 NPs were used as an ideal platform for microporous ZIF-67 growth, aiming to create an efficient heterogeneous catalyst with magnetic separation for the activation of peroxymonosulfate (PMS) to expeditiously degrade ciprofloxacin (CIP) antibiotics. The catalytic activity of the proposed nanocomposite was systematically evaluated with several operational factors, such as nanocatalyst and oxidant dosage, initial pH, co-existing anions, and the stability of the catalyst. Furthermore, scavenging technique and electron spin resonance (ESR) demonstrate that the sulfate and hydroxyl radicals play a major role in the degradation process. The findings indicate that ZIF-67/Fe3O4 nanocomposite is a greener and more suitable option for large scale applications and creates new insights into the removal of contaminants from the ecosystem.

- **Keywords:** Advanced oxidation processes; ZIF-67/Fe3O4; Core-shell nanocomposite; Antibiotics; Peroxymonosulfate

Natália Ueda Yamaguchi, Luís Fernando Cusioli, Heloise Beatriz Quesada, Maria Eliana Camargo Ferreira, Márcia Regina Fagundes-Klen, Angélica Marquetotti Salcedo Vieira, Raquel Guttierres Gomes, Marcelo Fernandes Vieira, Rosângela Bergamasco. *A review of Moringa oleifera seeds in water treatment: Trends and future challenges*. Pages 405-420.

The use of Moringa oleifera (MO) for cleaner processes in water treatment has been proposed to treat raw water for low-income locations for its abundant availability, low cost, reduced by-product generation, biodegradability, non-toxicity and multifunctional behavior. This review analyzed studies that used MO seeds in coagulation-flocculation processes, identifying the main proteins that presented coagulant activity. It was concluded that its most viable application would be as flocculation aid, since it was possible to reduce the concentration of the chemical coagulant with good removal results. Regarding the use of MO as adsorbent, studies could verify its potential to remove several water contaminants, such as pesticides, dyes and pharmaceuticals. Moreover, hybrid treatments have been investigated, however, a research gap could be verified regarding studies on pilot scale, which are fundamental for verifying the viability in water treatment plants. In this sense, the main trends, challenges and recommendations for further studies were assessed regarding the sustainable application of MO seeds in water treatment.

- **Keywords:** Moringa oleifera; Natural coagulant; Low-cost adsorbent; Water treatment plant; Water pollution

Syeda Zohra Halim, Noor Quddus, Hans Pasman. *Time-trend analysis of offshore fire incidents using nonhomogeneous Poisson process through Bayesian inference*. Pages 421-429.

Incident trend analysis has been important in the past for understanding how a system has been performing over time. The system can refer to a particular equipment, facility or organization and its performance can be monitored in terms of numbers or rates of failures, incidents or events over time. A good trend analysis leads to better projections into the future, enabling a more accurate prediction of future incidents or failures. In most cases however, it is generally assumed that incident or failure rates remain constant over time and the same value of the rate is used in all estimations. This study uses data of past offshore fire incidents in the Gulf of Mexico to predict future incidents and shows that such an assumption can fail to provide accurate predictions. The data is normalized to account for the year-to-year variation in operation and shows how using a nonhomogeneous Poisson process (NHPP) assumption, where failure rate is a function of time, enables a better understanding of performance, and can be used to predict future incidents more accurately. This will help regulatory bodies to understand whether operation in the Gulf of Mexico has been improving or not and to take proactive measures before the next fire incident occurs.

- **Keywords:** Offshore fire incidents; Time trend analysis; Bayesian inference; Nonhomogeneous Poisson process; Power law process

Chunhong He, Cuiping Yan, Cuiying Tang, Mei Huang, Ling Ren, Mingxing Zhang. *Nitrogen pulse jet cleaning of the pleated filter cartridge clogged with adhesive hygroscopic dusts*. Pages 430-438.

The pleated filter cartridges are widely used in industrial production to control particulate emissions and recover valuable particulate matter, where pulse jet cleaning is a major method for filter regeneration. However, for strong hygroscopic and adhesive dust such as Polyacrylamides (PAM), during pulse-jet cleaning the compressed air forms a low temperature zone at the nozzle and will release water to the environment, causing the

particles to adhere on the filter after absorbing moisture, resulting in ineffective filter regeneration. Therefore, a higher cleaning pressure or other methods are required to clean the filter surface. In this article, we have proposed a method to collect adhesive dust using dry gas injection and verified its feasibility through pilot experiments. The compressed air injection source was replaced with nitrogen, the curve of system pressure drop shows that nitrogen has good performance in the peeling of adhesive dust from the surface of the pleated filter cartridge. This highlights the effect of the moisture content in the cleaning compressed air on the regeneration of filters clogged with adhesive hygroscopic particles. Therefore, the feasibility of the nitrogen injection was validated, which provides a basis for the future systematic research of industry to collect adhesive dust.

- **Keywords:** Pleated filter cartridge; Adhesive dust; Pulse jet cleaning; Dry gas source; Polyacrylamides dust peeling off

Chaoran Wan, Qiang Xie, Jinchang Liu, Dingcheng Liang, Xiaoqing Huang, Huabing Zhou, Yuegang Tang, Deqian Liu. *Pilot-scale combined adsorption columns using activated carbon and zeolite for hazardous trace elements removal from wastewater of entrained-flow coal gasification*. Pages 439-449.

When entrained-flow gasification technology is applied on a large scale, the release of hazardous trace elements (HTEs) from the use of coal in gasification poses a potential threat to environmental and human health. An adsorption method combining granular activated carbon (GAC) and zeolite as adsorbents to remove the HTEs is proposed. A pilot-scale experiment proved that this method can effectively remove HTEs, especially, the removal rate for mercury and beryllium achieved 99%. Additionally, adsorption studies using GACs were conducted through laboratory batch experiments employing several kinetic and isotherm models. The results show favorable levels of mercury, arsenic, and beryllium adsorption by GAC. GAC derived from low rank bituminous coal has the good comprehensive adsorption performance of HTEs. Langmuir presented the best fit of arsenic and beryllium adsorption, and Freundlich presented the best fit of mercury. The kinetics studies showed that experimental data follow Pseudo-second order. Zeolite's capacity for ion exchange greatly affects its adsorption performance, which supplements the adsorption capacity of GAC for metal and metalloid ions. This study provides an approach that is fast, and easily integrates with existing processes for removing HTEs in entrained-flow coal gasification wastewater.

- **Keywords:** Entrained-flow coal gasification; Wastewater; Hazardous trace elements; adsorption; granular activated carbon; Zeolite

Alessandro Estarque de Oliveira, Vádila Giovana Guerra. *Electrostatic precipitation of nickel (II) oxide and sodium chloride nanoparticles: Operating conditions promoting sputtering with electro-fluid dynamics analysis*. Pages 450-459.

Erosion of metallic electrodes by sputtering is undesirable in electrostatic precipitators and must be avoided. This work reports the operational variables promoting sputtering, the applied voltage (−8.5 to −13.0 kV) and the air velocity (3.3 to 9.9 cm s−1), during the collection of NiO and KCl particles with a dry, wire-plate electrostatic precipitator, using electro-fluid dynamics analysis to evaluate the influence of the ionic flux on the sputtering. For the conditions evaluated in this work, the exclusive removal of NiO particles occurred at velocities of 9.9 cm s−1 (at applied voltages from −8.5 to −10.0 kV) and 3.3 cm s−1 (at −8.5 kV). Other operational conditions favored sputtering, causing the release of nanoparticles (median sizes of 10–25nm) from the device. The parameters of the particle size distribution were related to the natural logarithm of the

electro-fluid dynamics parameters, with coefficients of determination of 0.98 and 0.95 for the median size of the particles and the geometric standard deviation, respectively.

- **Keywords:** Electrostatic precipitation; Metal oxide nano-aerosols; Electro-fluid dynamics; Sputtering; Nano-aerosol production

Alex Kummer, Tamás Varga. *What do we know already about reactor runaway? a review*. Pages 460-476.

Nowadays, reactor runaway is still a crucial phenomen from the safety viewpoint. About 120 scientific journal articles are published every year in the last decade in which thermal runaway is a keyword. The possible cause and consequences of reactor runaway are adressed where the worst case is the explosion of the reactor. Prevention steps to avoid the development of thermal runaway include the appropriate design of the reactor, the operation strategy and an early warning detection system. The available assessment methods for thermal risk analysis are addressed in detail. Reactor runaway criteria can indicate early the thermal runaway, which criteria are addressed in this review in detail under three classes: geometry-, sensitivity-, and stability-based runaway criteria. Operation strategy of semi-batch reactors can be designed by calculating Westerterp-diagram whose evolution is cleary presented. Significant works on the field of the reactor design, operation and reactor safety are collected and evaluated. Finally possible further research areas are suggested to improve our knowledge about thermal safety, such as investigating parameter uncertainty in runaway indication or optimize the safety actions to moderate the consequences of runaway.

- **Keywords:** Runaway prevention; Thermal safety; Early warning system; Process safety; Thermal risk; Safety boundary diagram

Manoj Datta, Mohit Somani, G.V. Ramana, T.R. Sreekrishnan. *Feasibility of re-using soil-like material obtained from mining of old MSW dumps as an earth-fill and as compost*. Pages 477-487.

The present study examines the feasibility of using the soil-like material (SLM), less than 4.75mm size, recovered by the mining of old waste from four municipal solid waste dumps of India as an earth-fill for embankments, low-lying areas, deep pits and as compost for horticulture, agricultural applications. This material constitutes 60−70% of the total excavated waste. The contamination levels of SLM for re-use as earth-fills were analyzed on the basis of heavy metals, organic content, soluble salts, and release of dark-colored leachate. The reuse feasibility of SLM as compost was assessed on the basis of nutrients levels (total organic carbon, nitrogen, phosphorous, and potassium), heavy metals, and physicochemical characteristics. All the obtained results were compared with the values reported in the literature, national and international regulatory guidelines as well as with the background soils. The presence of high levels of organic matter, heavy metals, and soluble salts indicate that the SLM requires treatment before off-site re-use or that specific design measures are must before placing it as earth-fill in embankments, low-lying areas, and deep pits. The study also reveals that the re-use of mined SLM as compost should be restricted to non-agricultural applications due to excess heavy metals after supplementing the total organic carbon.

- **Keywords:** Aged MSW; Contaminants; Landfill mining; Old dumps

I. Salmerón, P.K. Sharma, M.I. Polo-López, A. Tolosana, S. McMichael, I. Oller, J.A. Byrne, P. Fernández-Ibáñez. *Electrochemically assisted photocatalysis for the simultaneous degradation of organic micro-contaminants and inactivation of microorganisms in water*. Pages 488-496.

This study presents the assessment of the performance of a photoelectrochemical reactor for the simultaneous degradation of organic microcontaminants (OMCs) and inactivation of bacteria in real surface water. Target OMCs were terbutryn, clorfenvinphos and diclofenac (500 µg l-1 each), and E. coli K12 (106 CFU mL−1) was used as the model microorganism. The reactor utilised a photoanode consisting of two Ti mesh electrodes anodised to give aligned self-assembled TiO2 nanotubes on the surface. Two cathode materials were investigated i.e. Pt and carbon felt. Higher E. coli inactivation rates were observed with electrochemically assisted photocatalysis (EAP) with a 2-Log Reduction Value (LRV) for Pt and 2.7-LRV in 2 h for carbon felt cathode, as compared to only a 0.8 LRV for photocatalysis (open circuit). For the simultaneous degradation of OMCs and inactivation of bacteria a 4.5-LRV was achieved in 90 min with applied potential and a carbon felt cathode. Similar degradation kinetics were observed for the OMC for both electrochemically assisted photocatalysis and photocatalysis (open circuit) with ca 70 % of the removal of the total OMCs in 60 min. Hydroxyl radical, H2O2 and chlorine generation were also evaluated to elucidate the mechanisms of degradation and disinfection. This work suggests that electrochemically assisted photocatalysis is more efficient than photocatalysis alone for the combined removal of OMCs and disinfection of water.

- **Keywords:** Carbon-felt cathode; Escherichia coli; Organic microcontaminants; Photoelectrocatalysis; TiO2 nanotubes photoanode; Water purification

Xana Alvarez, Ángeles Cancela, Adrián Rodríguez, Enrique Valero, Ángel Sanchez. *Green filters of Eucalyptus globulus for microalgae harvesting from freshwater reservoir and reuse of biomass harvested for pellet production*. Pages 497-504.

Filtration was used for the separation of microalgae from water collected at the reservoir of a Baxe, in north-western Spain, where cyanobacterial blooms are known to occur. The barks of Eucalyptus globulus were used as bed filters. Filters were made with compacted and non-compacted barks of 0.5, 1 and 2 g. Filtration of water with compacted barks showed the best results with yields of 43.12, 76.85 and 63.67 % for the different weights. The microalgae obtained and the vegetation filters were used for the manufacturing of pellets to be used as fuels. Their energy potential was studied according to different parameters such as calorific value, humidity, volatile matter and ash content, to verify the requirements for the use of pellets as fuel in biomass boilers met the criteria according to UNE Standards. These pellets meet the requirements of UNE standards established and could, therefore, be used in boilers as biofuels. Obtaining a high heating value above to 15.00 MJ/kg, greater than 17.00 MJ/kg for all samples except the pellet sample with only microalgal biomass. The samples have a lower ash content of (10 %), with the exception of the microalgae pellet without eucalyptus bark (13.67 %). The use of Eucalyptus bark is a feasible option for the separation of microalgae in aquatic ecosystems. The next step would be to carry out the experiments on a large scale in a reservoir with eutrophication problems, to test if it works correctly under different conditions. Although the aim of obtaining pellets for boilers does not pursue an economic or commercial objective, the results obtained were promising. This would help towards reducing forest waste and as consequence, reducing environmental pollution.

- **Keywords:** Microalgae; Filtration; Bloom; Pellet; Eucalyptus globulus

Jacqueline Bravo-García, Brenda Huerta-Rosas, Eduardo Sánchez-Ramírez, Juan Gabriel Segovia-Hernández. *Sustainability evaluation of intensified alternatives applied to the recovery of nylon industry effluents*. Pages 505-517.

Production pathway sustainability assessment is an important step in promoting sustainability characteristics during early process design. This work proposes distillation intensified alternatives for the recovery of nylon industry effluents. The waste stream contains n-pentanol, cyclohexanone, and cyclohexene oxide (light oil). These products in their pure state are high added-value products. The generation of intensified alternatives is based on the inclusion of thermally coupling, column section movement, and column section elimination. All the alternatives are evaluated in various metrics that guarantee the sustainability of the process; Mass Intensity, E-Factor, Greenhouse Gas Emissions, Total Annual Cost, Controllability, and Inherent Safety. As a result, the intensified alternative with a thermal coupling turned out the most balanced process in light of sustainability indicators with energy requirements of 4.87 MJ/kgproduct and important improvement in sustainability indexes.

- **Keywords:** Waste nylon treatment; Sustainable process; Intensified processes; Circular economy; Green processes

M.S. Gad, A.S. El-Shafay, H.M. Abu Hashish. *Assessment of diesel engine performance, emissions and combustion characteristics burning biodiesel blends from jatropha seeds*. Pages 518-526.

The consumption rise and environmental impact of diesel fuel led to the use of non-edible oils as alternative fuels. Different extraction processes as screw, soxhlet, solvent and hydraulic were investigated to show their effects on the properties and fatty acid composition of the oil from Egyptian jatropha seeds. Screw press extraction was characterized because of its higher oil yield and improved properties. Biodiesel was blended with diesel oil in volumetric ratios of 20, 40, 60, 80 and 100 % as B20, B40, B60, B80 and B100. Tests were performed at 75 % of the engine load and different engine speeds. The maximum decreases in output brake power and volumetric efficiency for B100 were 27 and 9 %, respectively but the maximum decrease in thermal efficiency for B100 was 33 % compared to diesel oil at 75% of engine load. The highest increase of NOX emission for B100 was 47 % at 75% of engine load about diesel oil. The maximum decline in smoke emission for B100 was 22 % about diesel oil at 75% of engine load. Cylinder pressures and heat release rate values of biodiesel blends were lower than crude diesel. Extracted oil by screw press was selected to be a biodiesel feedstock because of its improved physical and chemical properties. Lower volume percentages of biodiesel up to 20 % are recommended as alternative fuels due to near performance, emissions and combustion characteristics of diesel oil.

- **Keywords:** Jatropha seeds; Biodiesel; Performance; Emissions; Combustion characteristics

Wei Wang, Junmei Tian, Zhijia Zhu, Chenmiao Zhu, Baojiang Liu, Chunyan Hu. *Insight into quinolones and sulfonamides degradation, intermediate product identification and decomposition pathways with the assistance of Bi2MoO6/Bi2WO6/MWCNTs photocatalyst*. Pages 527-546.

A facile, efficient, precise and reliable method based on liquid chromatography-tandem mass spectrometry (HPLC-MS/MS) was established to separate and determine two typical quinolone antibiotics (ofloxacin and lomefloxacin) and two typical sulfonamide antibiotics (sulfadimeisoxazole and sulfadimidine). The photocatalytic degradation effects, identification of intermediate products and decomposition pathways of these four antibiotics degraded by Bi2MoO6/Bi2WO6/MWCNTs composite catalyst were analyzed using the developed HPLC-MS/MS method. It was found that all four antibiotics can be synchronously decomposed with the ultrahigh removal rates of above 95 %. Three main degradation reactions of quinolones were detected: the decarboxylation of quinolones,

the ring opening reaction of piperazine and the defluorination of C–F. The main decomposition reactions of sulfonamides included the sulfonamide bond (SN) breaking at the active sites, the oxidation of the amino acids on the benzene rings, and the substitution and oxidation ring opening reaction of pyrimidine. This study not only developed a detailed isolation and identification method for the degradation pathways and mechanisms of mixed pharmaceutical pollutants, but also provides a superb photocatalyst for the removal of multiplex pharmaceutical pollutants.

- **Keywords:** Composite photocatalyst; Photocatalytic degradation; HPLC-MS/MS; Quinolones and sulfonamides antibiotics; Degradation pathway

Zhenhua Wang, Kuibin Zhou, Le Zhang, Xuan Nie, Yueqiong Wu, Juncheng Jiang, Anne Simone Dederichs, Lu He. *Flame extension area and temperature profile of horizontal jet fire impinging on a vertical plate*. Pages 547-558.

Impinging jet fire of high exit momentum is frequently reported to induce the domino effect in industry fires. Less literature is available for the flame extension area and temperature distribution over a vertical plate impinged by the horizontal jet flame. Thus, this paper conducts a systematic experiment to reveal the effect of nozzle exit velocity, exit diameter and exit-plate spacing on the horizontally impinging jet fire. Experimental observation shows the evolution of flame pattern and color with an increase of exit velocity and a decrease of exit-plate spacing. The flame extension area induced by the horizontal jet flame impingement was measured by a novel method that combines the picture processing technique and the thermal imaging technique. By physical analysis, a new correlation coupling the turbulent Karlovitz stretch factor and the ratio of nozzle exit diameter to exit-plate spacing, was developed for the flame extension area of both horizontally and vertically impinging jet fire. The variation of maximum temperature in the impinging zone with the exit-plate spacing still fits the classic correlation of centerline temperature in the continuous and intermittent flames. However, the horizontally impinging jet fire plume holds a shorter intermittent flame region due to the flame upward bending. It is found that the temperature profile holds a big difference in the upward and downward directions along the vertical plate. A new uniform correlation, with the plume radius as the characteristic length scale, is proposed to well collapse all the temperature data in the impinging zone.

- **Keywords:** Jet fire; Impingement jet; Flame extension; Flame temperature; Vertical plate; Exit velocity

Georgy Lazorenko, Anton Kasprzhitskii, Faiz Shaikh, R.S Krishna, Jyotirmoy Mishra. *Utilization potential of mine tailings in geopolymers: Physicochemical and environmental aspects*. Pages 559-577.

The mining industry produces a large amount of mine waste rock and tailings, which pose a severe threat to the environment. The most common way for the disposal of these industrial wastes is dumping at sites, which contributes to soil degradation and water pollution, and also covers the useful land. Recycling of mine tailings (MTs) in raw material - intensive applications presents a good alternative to manage the waste generated from mining and mineral processing industries. The geopolymer technology provides a green solution to the utilization of MTs, avoiding its negative environmental impacts. This paper is the first part of the review which summarizes the physicochemical and environmental aspects of different types of MTs, as well as the technological aspects of the preparation of geopolymers (GPs) based on them. The work scrutinizes potential environmental and socio-economic risks of the mining industry associated with the accumulation of tailings. The issues of MTs toxicity that should be taken into account when developing methods for disposal of tailings in geopolymers are touched upon. The

features of the chemical and mineral composition of tailings used in geopolymers, as well as their physical properties, are systematized and scrutinized. Methods of utilizing MTs as precursors of GPs or aggregates described in the scientific literature, as well as general patterns of the geopolymerization process are discussed. Finally, the key issues in this area that require additional research are highlighted.

- **Keywords:** Geopolymers; Alkali-activated materials; Mine tailings; Industrial waste

Yanan Qian, Wei Xu, Jin-Hui Zhan, Xuewu Jia, Fan Zhang. *Atomic insights into the thermal runaway process of hydrogen peroxide and 1,3,5-trimethybenzene mixture: Combining ReaxFF MD and DFT methods*. Pages 578-588.

The explosive hazard of hydrogen peroxide (H2O2) and organics mixtures had drawn much attention, but the mechanism is still unclear. In this work, the atomic insights into the thermal runaway process of H2O2 and 1,3,5-trimethylbenzene (TMB) mixture was conducted using a new approach of combining reactive molecular dynamics (ReaxFF MD) and density function theory (DFT). The detailed reaction pathways were obtained through ReaxFF MD. The kinetic and thermal properties of main reaction steps were examined by DFT. This work divided the thermal runaway process into two stages. In stage I, H2O2 molecules were decomposed first to generate ·OOH and ·OH free radicals. The ·OH radicals induced the initial oxidation of TMB molecular through H-abstraction and ·OH-combine reaction steps with the highest thermal energy of 921.76 kJ/mol released, evoking the opening and cracking of benzene ring. In stage II, once the generated small molecules were further oxidized, the reactions showed a runaway for the massive thermal energy released, which explains the mechanism of larger potential risk of H2O2-organics mixture. Notably, ·OH is the most crucial free radical carrier for the whole reaction process, the explosion hazard will be inhibited or weakened if the concentration of ·OH radical is controlled. It is expected that this work will help researchers and industrial practitioners to better understand the intrinsic thermal hazard of H2O2-organics, and provide valuable guidance for the further development of efficient explosion suppression methods.

- **Keywords:** Hydrogen peroxide; Organics; ReaxFF MD; DFT calculation; Thermal runaway

Mariam N. Soliman, Fatima Z. Guen, Somaya A. Ahmed, Haleema Saleem, Mohd Junaid Khalil, Syed Javaid Zaidi. *Energy consumption and environmental impact assessment of desalination plants and brine disposal strategies*. Pages 589-608.

Nowadays, desalination plants are considered as tools to utilize water from different natural resources such as seawater and brackish water. Globally, the number of desalination plants are increasing to achieve the high demand for fresh water to be used for human consumption, industrial activities, and public services. However, the brine discharged will have detrimental effect on the marine environment, and thus the brine should be reused, treated, or discharged properly. The present study aims to give a comprehensive insight into the current development of the desalination process through examining the different technologies available, energy consumption, water production costs of these technologies and the brine water characteristics. Several brine disposal strategies are analysed here and compared to evaluate their effectiveness and drawbacks. The potential usages of brine are also carefully examined. Also, we discuss the zero-liquid discharge (ZLD) method, its benefits, challenges, environmental and operating characteristics, and the current progress of research in this field. Ultimately, the future research and development strategies for the concentrate management are

briefly analysed. It was noted that the ZLD process is very significant to the environment in terms of reducing the pollution caused by discharged brine and achieving sustainability.

- **Keywords:** Seawater desalination; Membrane technologies; Thermal technologies; Brine disposal; Zero liquid discharge (ZLD)

Jovana Perendija, Zlate S. Veličković, Ilija Cvijetić, Steva Lević, Aleksandar D. Marinković, Milena Milošević, Antonije Onjia. *Bio-membrane based on modified cellulose, lignin, and tannic acid for cation and oxyanion removal: Experimental and theoretical study*. Pages 609-625.

Two optimized methods, based on epoxy-amino reactivity of the Cellulose fibres (Cell) modified with diethylenetriamine (Cell–DETA), (3-Glycidyloxypropyl)trimethoxysilane (Cell-Glymo), Lignin modified with epichlorohydrine (EL) and Tannic acid (TA), as an additional crosslinker, were developed for the production of the bio-renewable Cell-EL and Cell-EL-TA membranes. The influences of pH, contact time, adsorbent dose, and temperature on adsorption performances were studied by batch adsorption tests. The calculated capacities: 53.9, 99.9, 97.8 and 63.5, 115.8, 127.5 mg g−1 for Ni2+, Pb2+, Cr(VI) using Cell-EL and Cell-EL-TA, respectively, were obtained from Langmuir model fitting at 25 °C. The thermodynamic parameters indicated spontaneous and low endothermic processes. The results of the kinetic study, i.e. pseudo-second-order (PSO) and Weber-Morris (W-M), suggest an intra-particle diffusion as a rate-limiting step. The semi-empirical quantum chemical calculations aided the analysis of the non-specific and specific adsorbent/adsorbate interactions and their contribution to the overall bonding mechanism. Membrane utility was confirmed by performing a bed column study. In general, three main environmental issues of the present study, biodegradability of the used membrane, desorption efficiency, and development of the technology for the effective effluent water treatment and safe disposal of by-products highly conform to the demand of integrated environmental management system applicability in practice.

- **Keywords:** Cellulose membrane; Batch and column study; Semi-empirical calculations; Sustainable development

Mohammad Javad Amiri, Alireza Faraji, Morteza Azizi, Bahareh Goudarzi Nejad, Mohammad Arshadi. *Recycling bone waste and cobalt-wastewater into a highly stable and efficient activator of peroxymonosulfate for dye and HEPES degradation*. Pages 626-641.

In view of the great demand for using sustainable, renewable, and widely available resources to generate catalysts for advanced oxidation processes (AOPs), bio-originated waste materials show great promise as an alternative to state-of-the-art materials that suffer from high cost and scarcity. In this paper, we modified the ostrich bone waste (OBW) with hydrogen peroxide (HP) to produce OBW/HP with excellent chemical and mechanical strength that can in one sweep recover valuable heavy metal ions like Co from industrial wastewater and provide a sustainable catalyst-OBW/HP@CoNP- to activate peroxymonosulfate (PMS) for the degradation of dyes. After treatment of OBW with HP and Co ions, the morphologies of OBW/HP and OBW/HP@CoNP completely changed-porous, fine and flat sheets appeared, and well-dispersed, stable spherical Co nanoparticles of 50−70 nm were generated, respectively. PMS-OBW/HP@CoNP system was able to remove several cationic and anionic dyes such as methylene blue (99.9 %), crystal violet (96.0 %), and congo red (76.0 %) within 120 min. As proof-of-concept applications, we prepared a membrane using a layer of OBW/HP@CoNP and a microreactor by encapsulating a water droplet within OBW/HP@CoNP shell, and found that the materials exhibit rapid kinetics to degrade MB within 30 s. In addition, the

degradation of HEPES as a representative organic buffer was also studied for the first time at pH 7.4 and the mechanism of HEPES removal (98 %) was elucidated by LC–MS. Finally, although the preparation of OBW/HP@CoNP does not release toxic and synthetic compounds into the water, shows many advantages as catalyst and membrane- which promising its applications in industrial-scale including low-cost, sustainability, high chemical and mechanical stability, no metal leaching, and superior effectiveness in activating PMS, and recyclability.

- **Keywords:** Dye degradation; Sulfate radicals; Cobalt; Ostrich waste bone; Renewable resource; Peroxymonosulfate

Reza Mahinroosta, Lalantha Senevirathna, Miao Li, Karthika KrishnaPillai. *A methodology for transport modelling of a contaminated site with perfluorooctane sulfonate due to climate interaction*. Pages 642-653.

In this study, a numerical model was developed to predict perfluorooctane sulfonate (PFOS) migration in a contaminated site due to precipitation and evapotranspiration over 100 years. The soil physicochemical properties including sorption isotherm characteristics were used to model PFOS transport (advection and dispersion), and attenuation (adsorption and decay) processes using the GeoStudio software. The model was calibrated using the results of a leachate test on a reconstituted contaminated soil specimen. The simulation of the contaminated site showed that in the current situation where the site is covered by a concrete slab, PFOS remains at the site beneath the concrete slab for a long time with decay being the dominant factor contributing to its reduction over time. It took several decades for PFOS to contaminate groundwater. The PFOS level in groundwater reached the threshold value for drinking water in 25 years and continued to increase in the long term, extending horizontally to an area up to five times the size of the contaminated site. This issue needs to be considered when digging boreholes for drinking water close to the contaminated site.

- **Keywords:** Contaminant transport; Climate interactions; Groundwater; Numerical modelling; PFAS; PFOS prediction

Zhen Cheng, Lei Ni, Junjie Wang, Juncheng Jiang, Hang Yao, Qiang Chen, Fusheng Cui, Wei Jiang, Shuliang Ye. *Process hazard evaluation and exothermic mechanism for the synthesis of n-butylmagnesium bromide Grignard reagent in different solvents*. Pages 654-673.

The synthesis of Grignard reagents, which are formed by the reaction of magnesium and organic halides (RX), is hazardous because of the highly exothermic nature of this reaction. In this work, calorimetry and infrared (IR) spectroscopy were used to identify the exothermic mechanism and process hazards for the synthesis of n-butylmagnesium bromide Grignard reagent (n-BuMgBr) in diethyl ether (DE), tetrahydrofuran (THF), 2-methyltetrahydrofuran (2-MeTHF), cyclopentylmethyl ether (CPME), and diethylene glycol butyl ether (DGBE). The latter three solvents were chosen by the substitution principle of the "inherent safety" design concept, which aims to reduce the risk of the target reaction in a fundamental manner. An EasyMax102 calorimeter was used to characterize the exothermic behavior of the reactions using isothermal and isoperibolic experiments carried out in a semi-batch glass reactor coupled with an IR probe to monitor changes in the species and concentrations during the reaction process. An adiabatic TAC-500A calorimeter was also used to understand the adiabatic decomposition behavior of the products obtained in the isothermal experiments under the worst-case (cooling failure and thermal runaway) scenario. Meanwhile, density functional theory calculations were performed to understand the reaction pathway and associated energies based on the experimental data. Further, the risk assessment of thermal runaway was analyzed using

a risk matrix and a Stoessel criticality diagram. The results indicate that the risk of the reactions when using 2-MeTHF, CPME, and DGBE are all class 1, making reactions in these solvents inherently safer than those using DE or THF, which were both class-3 risks. These findings provide further evidence that 2-MeTHF, CPME, and DGBE are safer than the typical solvents used for the industrial production of Grignard reagents.

- **Keywords:** Grignard reagent; Exothermic mechanism; Solvents; Inherent safety; Thermal runaway; Risk assessment

Oswaldo Gomes Júnior, Maria Gabriela B. Santos, Arlene B.S. Nossol, Maria Clara V.M. Starling, Alam G. Trovó. *Decontamination and toxicity removal of an industrial effluent containing pesticides via multistage treatment: Coagulation-flocculation-settling and photo-Fenton process*. Pages 674-683.

This paper evaluates the combination of coagulation-flocculation-settling and photo-Fenton for the decontamination of a real effluent containing ametrine ([AMT]=403mg L−1), atrazine ([ATZ]=2153mg L−1), imidacloprid ([IMD]=2936mg L−1) and tebuthiuron ([TBT]=3354mg L−1) and which is generated during the manufacturing process of pesticides. Physicochemical treatment (coagulation-flocculation-settling) was tested using different concentrations of Al(NO3)3 and Fe(NO3)3. No significant removal was achieved using Al(NO3)3 as coagulant while best results were obtained via coagulation with Fe(NO3)3 (99 % removal of color and turbidity). Pesticides remaining in the supernatant after coagulation-flocculation-settling stages were removed via photo-Fenton under black-light or solar irradiation. 82–95 % removal of target pesticides were obtained after photo-Fenton treatment (2mmol L−1 of FeOx, 5463mgL−1 of H2O2) using black-light lamps (400kJ m−2). Solar irradiation improved the degradation of target pesticides (>99 %) leading to concentrations below quantification limits (<0.1mg L−1; 400kJ m−2). Effluent acute toxicity (Vibrio fischeri) was reduced from 100 % to 43 % after solar photo-Fenton. Highly oxidized compounds were formed as confirmed by an increase in average and carbon oxidation states. Preliminary costs calculated for the proposed treatment indicated that $ 349 may be saved per m3 of treated effluent when compared to costs associated to the conventional treatment for this effluent (incineration).

- **Keywords:** Advanced oxidation process; Ametrine; Atrazine; Imidacloprid; Tebuthiuron; Solar irradiation

Pantea Moradi, Majid Saidi, Ali Taheri Najafabadi. *Biodiesel production via esterification of oleic acid as a representative of free fatty acid using electrolysis technique as a novel approach: Non-catalytic and catalytic conversion*. Pages 684-692.

In the present study, production of biodiesel from biomass containing free fatty acids has been evaluated through electrolysis method as a novel efficient technique, in absence and presence of alkaline and acidic catalysts at mild operating condition. The impact of operating parameters such as voltage (10−30 V/cm), reaction time (1−3 h), methanol to oil molar ratio (10:1−40:1), acetone to methanol molar ratio (0:1−0.5:1), NaCl concentration (0−0.045 M) and catalyst type and loading on the process performance have been investigated in term of biodiesel production yield. The achieved results indicate that the biodiesel production yield using electrolysis method is about 42 % at voltage of 20 V/cm, reaction time of 2 h, NaCl concentration of 0.015 M, methanol to oil molar ratio of 20:1, acetone to methanol molar ratio of 0.25:1 and without presence of catalyst, whereas it is improved to 52 % and 95 % in the presence of 5.6 wt.% of KOH and 13 wt.% of H2SO4 as catalyst, respectively. The determined physicochemical properties of the synthesized biodiesel via electrolysis method incorporating density,

kinematic viscosity, cetane index, Iodine value and cloud point properties satisfy the main fuel standard criteria. The cetane index of synthesized biodiesel using electrolysis method is 57.3.

- **Keywords:** Biodiesel; Electrochemical method; Free fatty acid; Fatty acid alkyl ester; Methyloleate

Federica Ricci, Giordano Emrys Scarponi, Elsa Pastor, Eulàlia Planas, Valerio Cozzani. *Safety distances for storage tanks to prevent fire damage in Wildland-Industrial Interface*. Pages 693-702.

Wildfire occurrence frequency is increasing worldwide, generating more and more concern, especially in Wildland-Urban interfaces (WUI) and Wildland-Industrial Interfaces (WII) areas. Wildfires approaching WII can cause severe damage to people and industrial assets. In these scenarios, storage tanks present in industrial installations are among the most vulnerable pieces of equipment, since they are usually located in the proximity of the plant boundary. If hazardous substances are stored, tank damage caused by the fire can lead to loss of containment and trigger technological accident scenarios, escalating the consequences. Preserving the integrity of this type of equipment in case of wildfires is of paramount importance. The present study proposes a stepwise methodology for the evaluation of safety distances between storage tanks and vegetation that may be affected by a wildfire. According to the available data on the wildfire, on the lay-out and on the tanks that are likely to be affected, the methodology provides safety distances that may be applied to design fuel-reduced fringes around the industrial facility. The methodology proposed represents a quantitative tool for the calculation of safety distances that can guide industrial managers and assist regulators in the definition of more reliable standards. The comparison of the safety distances resulting from the present study with regulations and guidelines currently in use in different countries rises concern about the possible underestimation of required safety distances in the case of severe wildfires.

- **Keywords:** NaTech; Wildfire; Major accident hazard; Wildland-urban interface; Fuel-reduced fringes; Storage tanks

Federica Ricci, Valeria Casson Moreno, Valerio Cozzani. *A comprehensive analysis of the occurrence of Natech events in the process industry*. Pages 703-713.

Natural events triggering technological scenarios (Natech events) are an increasing concern for regulatory authorities and industry, in particular in areas prone to natural disasters. A comprehensive analysis of the occurrence of Natech scenarios affecting the process industry is presented. A dataset of 9100 past accidents that took place in the last 70 years was compiled and analysed, with the aim of understanding the trend of Natech events, their geographical distribution, the final technological scenarios, and the associated consequences in terms of human losses and asset damages. Meteorological events, such as storms, extreme temperatures and lightning were found to be the main trigger of Natech scenarios (86 %). Despite the difficulty in collecting homogeneous data worldwide, an increasing number of Natech events over the time is observed. Moreover, specific increases in the occurrence of Natech events correspond to the occurrence of severe natural disasters as the devastating hurricanes that affected the Gulf of Mexico in recent years. The societal risk curve associated to Natechs was calculated, evidencing the relevance of extremely severe accidents (> 100 deaths). The analysis of the dataset also allowed building quantified event trees for the evolution of Natech scenarios. Specific ignition probability values for Natech events were estimated.

- **Keywords:** Natech; Major accident hazard; Chemical and process industry; Event tree; Societal risk

Hao Chen, Jingjing He, Zhanming Chen, Limin Geng. *A comparative study of combustion and emission characteristics of dual-fuel engine fueled with diesel/methanol and diesel–polyoxymethylene dimethyl ether blend/methanol*. Pages 714-722.

In this study, a comparative study of the combustion characteristics and performances of a dual-fuel engine fueled with diesel/methanol and diesel–polyoxymethylene dimethyl ether blend/methanol was conducted. All the experiments were conducted on a heavy-duty common rail diesel engine at an engine speed of 1800 r/min. The engine loads were fixed at low, medium, and heavy loads, with the brake mean effective pressure at 0.42 MPa, 0.7 MPa and 0.9 MPa, respectively. Methanol substitution ratio (MSR) was defined as the torque output contributed by methanol to the total torque output, and in this study, three MSRs (0 %, 20 %, and 40 %) were defined. Diesel–polyoxymethylene dimethyl ether (PODE) blend was defined as P50 (50 % diesel and 50 % PODE by volume) to clarify the effect of PODE addition on engine performance. The results showed that the dual-fuel engine fueled with P50/methanol had a higher peak cylinder pressure, lower first peak heat release rate (HRR), and higher second peak HRR than the dual-fuel engine fueled with diesel/methanol. Both the ignition delay and combustion duration of the dual-fuel engine decreased when the pilot fuel injection changed from diesel to P50. Moreover, both NOx emissions and particulate matter produced by the P50/methanol engine were lower than those produced by the diesel/methanol engine for the specific MSR and engine load.

- **Keywords:** Dual-fuel; Diesel/methanol; P50/methanol; Combustion characteristics; Emissions

Samy Yousef, Justas Eimontas, Sharath P. Subadra, Nerijus Striūgas. *Functionalization of char derived from pyrolysis of metallised food packaging plastics waste and its application as a filler in fiberglass/epoxy composites*. Pages 723-733.

Char derived from pyrolysis of plastic wastes represents about 20 wt.% of the released pyrolysis products. In order to maximize the economic benefits and applications of this fraction, this research aims to refine and reprocess char derived from plastic waste into carbon particles, then using it as a micro-filler material for light material applications. The experiments were performed on char derived from pyrolysis of metallised food packaging plastics wastes (MFPWs) that represent the most complicated part in plastic waste, and their char is usually loaded with aluminium elements. The experiments started with treating MFPWs in pyrolysis plant with a capacity of 250 g, followed by separation of char from other pyrolysis products. The derived char was exposed to a milling process followed by a leaching process to separate Al fraction and other heavy metals. The liberated carbon particles were exposed to functionalization process to remove any contamination and amorphous impurities. The functionalized carbon black particles in the form of spherical microparticles (FBC: 0.25, 0.5, 0.75, and 1 wt.%) were used to enhance the mechanical impact, and thermal behaviour of fiberglass/epoxy composite laminates. The composite panels were prepared using vacuum-assisted resin transfer and curing processes. The morphology and the composition of FBC were examined using SEM-EDS and FTIR. Also, SEM and Optical Microscope were used to observe dispersion of FBC, microstructure, impact mechanism, and surface morphology of the fabricated matrix. The mechanical and impact properties of the panels were tested according to ASTM-D7025 and ISO 6603-2 standards, respectively. Finally, thermal behaviour of the panels was studied using a thermogravimetric analysis. The results showed that 0.75 wt.% of FBC were enough to improve the modulus of elasticity of panels by ~22 %, compared to a pure sample. In addition, thermal stability and energy impact absorption at the same concentration of FBCs were improved by 21 % (in the main decomposition zone) and 38 %, respectively.

- **Keywords:** Plastic waste; Metallised food packaging plastics; Pyrolysis; Char; Carbon black particles; Fiberglass Epoxy Composites

Vicent Hernández-Chover, Águeda Bellver-Domingo, Francesc Hernández-Sancho. *The influence of oversizing on maintenance cost in wastewater treatment plants*. Pages 734-741.

Management of Wastewater Treatment Plants (WWTPs) is a complex process, not only from a technical point of view but also from an economic point of view. There are several factors that influence the wastewater treatment process and can cause an increase in management costs. One of these factors is the treatment capacity, in particular the WWTPs' oversizing problem. The difference between the design population equivalent (p.e.) and the actual p.e. treated generates imbalances in the wastewater treatment process costs. This paper analyses the influence that oversizing has on the maintenance costs for WWTPs in the Valencia region (Spain). Through an econometric approach, the behaviour of WWTPs including the oversizing variable has been modelled. Specifically, maintenance cost functions have been obtained to model the variability of maintenance costs according to oversizing influence. To date, this approach has not been considered in the published literature, reinforcing the novelty of this work. Results verify the significant influence of oversizing on maintenance costs in WWTPs. Modelling proposed in this work acts as an effective tool for WWTP managers to identify both the maintenance cost trend and how far the WWTP is from the design p.e. Likewise, results confirm the fact that WWTPs should work close to their design p.e. to improve the efficiency of the wastewater treatment process, reducing WWTPs' costs.

- **Keywords:** Asset management; Wastewater facilities; Design; Maintenance cost; Sizing; Oversizing

Ushtar Arshad, Syed Ali Ammar Taqvi, Azizul Buang. *Modelling of the minimum ignition temperature (MIT) of corn dust using statistical analysis and artificial neural networks based on the synergistic effect of concentration and dispersion pressure*. Pages 742-755.

Corn dust is a highly energetic substance and frequently found in the food manufacturing industries. It not only poses occupational safety hazards such as suffocation or lung disorders for exposed persons but is often extremely explosible in ignition sensitive environment. This probability of explosion can be assessed and minimised with in-depth knowledge of controlling parameters/physical properties that trigger the ignition. This research takes into account the minimum ignition temperature (MIT), which is the control parameter for explosion risk assessment. MIT relies on multiple factors, such as moisture content, particle size, dust concentration, dispersion pressure, humidity and environmental temperature. In this study, the ignition of corn dust clouds was analysed using a Godbert Greenwald furnace for different combinations of dispersion pressure and concentrations. Test findings revealed that the minimum ignition temperature rises with a decrease in particle size. However, the minimum ignition temperature decreases with increased dispersion pressure and concentration until a specific value known as optimal value for ignition. Moreover, this work focuses on a statistical approach of polynomial surface fitting to forecast the MIT based on the combined impact of concentration and dispersion pressure on MIT for corn dust in a real-time experiment. The minimum value of the Bayesian Information Criterion (BIC) was used to select the most appropriate polynomial model due to its authenticity and strong reputation. An artificial neural network (ANN) is also used as a predictive tool to develop a model that can forecast the MIT with a defined combination of dispersion pressures and corn dust concentrations. As soon as an appropriate estimation of this minimum ignition temperature of the combustible dust is confirmed, it is possible to ensure that the temperatures of the surrounding hot surfaces do not rise to that point to prevent the explosion. The predictive

results obtained from ANN were found to be good when compared with the polynomial surface fit. Several models with different numbers of neurons have been trained with different transfer functions. For the training, validation, and test phases, R values are around 1.0, i.e., 0.9863, 0.9930, and 0.9893, respectively. The overall R value was 0.9875 for the proposed network. The findings were considered to be acceptable as the overall value of R was close to 1.0. The network obtained sufficiently comparable findings with the research conducted by Kasalova and Balog.

- **Keywords:** Minimum ignition temperature; Corn dust; ANN modelling; Gobert-Greenwald furnace

Zahra Shabani, Mohammad Kahrizi, Toraj Mohammadi, Norollah Kasiri, Soleyman Sahebi. *A novel thin film composite forward osmosis membrane using bio-inspired polydopamine coated polyvinyl chloride substrate: Experimental and computational fluid dynamics modelling*. Pages 756-771.

A novel low-cost polyvinyl chloride (PVC) membrane was synthesized by phase inversion and fast and facile bio-inspired technique was used for substrate modification of a thin-film composite (TFC) forward osmosis (FO) membrane. Using DI water as feed solution (FS) and 1 M NaCl as draw solution (DS), water flux (WF) ranging from 4.15 to 15.95 LMH and reverse salt flux (RSF) ranging from 0.87 to 3.50 gMH were produced when the dope polymer solution concentration decreased from 17 to 10 wt%. Then, the substrate with 10 wt% PVC was selected for modification and the substrate was coated by dopamine (DA) solution for 1 and 3 h to enhance the membrane hydrophilicity and facilitate interfacial polymerization. Compared to the pristine membrane, the 1 h polydopamine (PDA) modified membrane displayed higher WF (18.90 LMH) and lower RSF (3.35 gMH). Whereas, for the longer coating time, WF decreased (9.70 LMH) due to the membrane surface pores blocking by the PDA layer. Finally, for understanding whether the experimental data can be supported by a theoretical model, the obtained experimental results were compared with a developed computational fluid dynamics (CFD) model and the results showed acceptable agreement with each other. The results of this work introduce a low-cost and facile approach for FO membrane fabrication by utilizing PVC polymer and PDA coating.

- **Keywords:** Polyvinyl chloride (PVC); Bio-inspired technique; Thin-film composite; Forward osmosis; Polydopamine

Ying Zhang, Beini Zhang, Yue Chen, Bihe Yuan, Wei Zhang, Sheng Shang. Effectiveness and mechanism of sodium phytate as a green inhibitor for the dust deflagration of lysine sulfate. Pages 772-787.

Lysine sulfate (LS) powder is at high risk of fire and explosion during its production, processing and storage. Considering its edible and nutritive values, the selection for its explosion inhibitor requires both excellent inhibition performance and environmental friendliness. The inhibition performance of a natural food additive of sodium phytate (SP) on LS dust deflagration is investigated by comparing it with ammonium polyphosphate (APP), which is a widely used flame retardant. The deflagration characteristics of LS mixtures with various mass fractions of SP and APP are recorded by high-speed photography and fine thermocouples. The combustion heat is tested by micro-scale combustion calorimetry. Thermal stability of samples are studied by using a synchronous thermal analyzer. The results show that the deflagration of LS dust is completely suppressed when the mass fractions of APP and SP increase to 2% and 8%, respectively. The corresponding inhibition mechanisms are proposed based on the dust deflagration macroscopic results and microcosmic analysis on thermal decomposition products and

residuals. These findings may provide a solution to reduce the probability and damage of dust explosions.

- **Keywords:** Lysine sulfate; Dust deflagration; Green inhibitor; Sodium phytate; Ammonium polyphosphate

Fei Sun, Ting-Ting Li, Hai-Tao Ren, Bing-Chiuan Shiu, Hao-Kai Peng, Jia-Horng Lin, Ching-Wen Lou. *Dopamine-decorated lotus leaf-like PVDF/TiO2 membrane with underwater superoleophobic for highly efficient oil-water separation*. Pages 788-797.

Oil and organic pollutants removal becomes an efficient solution to dispose of industrial oily and textile dye wastewater. This study proposes a lotus leaf-like bionic nanofibrous membrane with underwater superoleophobic for highly efficient oil-water separation. Papillary structure of the bionic membrane is formed by electrospraying of PVDF and TiO2 solutions on the surface of beaded-structure PVDF/TiO2 membrane. Dopamine is then decorated on the resultant PVDF/TiO2 membrane by in situ polymerization to be with hydrophilic-underwater oleophobic property for highly efficient oil-water separation. This bionic membrane has > 99 % oil-water separation efficiency, and high flux of 1389 ± 67 L m−2 h−1. Its contact angle of underwater petroleum ether and dichlomethane reaches 155° and 152°, respectively. Moreover, it has excellent water transport capacity, photocatalytic property, as well as high separation efficiency and flux even after 5-cycle filtration. This bionic nanofibrous membrane will become a promising candidate in clean production, industrial oil/water separation, water purification and efficient liquid transmission.

- **Keywords:** Bio-inspired; Papillae structure; Electrospraying; Dopamine; Oil/water separation

Gizele D. Silva, Eduardo O. Marson, Letícia L. Batista, Carlos Ueira-Vieira, Maria Clara V.M. Starling, Alam G. Trovó. *Contrasting the performance of photo-Fenton at neutral pH in the presence of different organic iron-complexes using hydrogen peroxide or persulfate as oxidants for naproxen degradation and removal of antimicrobial activity*. Pages 798-807.

This is the first study to compare the combination of different iron complexes (Fe3+-oxalate (FeOx), Fe3+-citrate (FeCit), Fe3+-nitrilotriacetic acid (FeNTA), Fe3+-ethylenediaminetetraacetic acid (FeEDTA) and Fe3+-ethylenediamine-N,N′-disuccinic acid (FeEDDS) with distinct oxidants (H2O2 and S2O82−) on the degradation of naproxen (NAP) via photo-Fenton. Experiments were performed in distilled water and in sewage treatment plant effluent and different Fe/organic ligand molar ratios, oxidant concentrations and radiation sources (black light and sunlight) were tested for each complex. Photo-Fenton at neutral pH was efficient for naproxen degradation in the presence of all iron complexes. Fe/ligand molar ratio was strongly affected by the ligand type, best results were obtained in the presence of Fe/EDDS (1:1) and Fe/NTA (1:1), Fe/EDTA (1:2), Fe/Cit (1:3) and Fe/Ox (1:12). Although NAP removal in distilled water was faster in the presence of H2O2 (max 20 kJ m−2 required) when compared to S2O82− (max 90 kJ m−2 required), better performance of S2O82− was observed in sewage treatment plant effluent. Antimicrobial activity was only observed in the presence of FeEDDS, yet it was eliminated after treatment in the presence of S2O82−. A critical comparison in terms of operational and electrical energy costs indicates that using FeCit complex with H2O2 is the most cost-effective alternative in both matrices.

- **Keywords:** Advanced oxidation processes; Environmental aqueous matrices; Escherichia coli; Iron complexes; Sewage treatment plant effluent

Carla S. Fermanelli, Liliana B. Pierella, Clara Saux. *Comparative study of zeolites matrices in bio-wastes pyrolytic valorization*. Pages 808-817.

Considering the importance of bio-wastes thermo-chemical conversion to fuel and platform molecules, three types of zeolites (ZSM-5, Beta and Y) were tested as heterogeneous catalysts. Peanut shell is a high volume agricultural waste. Its pyrolysis mediated by different catalysts was evaluated. The effect of the zeolite matrix over the bio-oil yield and products selectivities was carefully considered. Fresh and used materials were widely characterized by XRD, FTIR, ICP and BET techniques. Pyrolysis reactions were done at 500 °C under N2 flow. The use of zeolites in biomass pyrolysis showed interesting results in terms of bio-oil composition. When H-ZSM-5 catalyst was employed, higher bio-oil yields and greater concentration of aromatic hydrocarbons and furans were obtained.

- **Keywords:** Bio-oil upgrade; Bio-waste; Peanut shell; Zeolite

Mohamed El Amine Ben Seghier, Behrooze Keshtegar, Mohammed Taleb-Berrouane, Rouzbeh Abbassi, Nguyen-Thoi Trung. *Advanced intelligence frameworks for predicting maximum pitting corrosion depth in oil and gas pipelines*. Pages 818-833.

The main objective of this paper is to develop accurate novel frameworks for the estimation of the maximum pitting corrosion depth in oil and gas pipelines based on data-driven techniques. Thus, different advanced approaches using Artificial Intelligence (AI) models were applied, including Artificial Neural Network (ANN), M5 Tree (M5Tree), Multivariate Adaptive Regression Splines (MARS), Locally Weighted Polynomials (LWP), Kriging (KR), and Extreme Learning Machines (ELM). Additionally, a total of 259 measurement samples of maximum pitting corrosion depth for pipelines located in different environments were extracted from the literature and used for developing the AI-models in terms of training and testing.Furthermore, an investigation was carried out on the relationship between the maximum pitting depths and several combinations of probable factors that induce the pitting growth process such as the pipeline age, and the surrounding environmental properties. The results of the proposed AI-frameworks were compared using various criteria. Thus, statistical, uncertainty and external validation analyses were utilized to compare the efficiency and accuracy of the proposed AI-models and to investigate the main contributing factors for accurate predictions of the maximum pitting depth in the oil and gas pipeline.

- **Keywords:** Oil and gas pipelines; Pitting corrosion; Maximum depth; Artificial Intelligence (AI); Global performance indicator (GPI); External validation

Amin el Aissami, Frans Snijkers. *Sustainable future technologies: A concept for risk assessment applied to chemical looping combustion installations*. Pages 834-845.

The applicability of the Safe-by-Design (SbD) concept was investigated during development of oxygen carriers (OCs) for Chemical Looping Combustion (CLC) installations; the newly developed OCs are complex, fluidizable metal-oxides. SbD assesses Health Safety and Environmental (HSE) risks at an early stage of product development. Hereto, the impact of the key parameters on safety of future industrial units were estimated with exposure simulations (solid pouring tests and modelling by similarity with commercial refining technology). The likelihood of health effects for workers exposed via inhalation was examined with in vitro tests, showing that particles of Mn-based OC have the potency to initiate an allergic reaction (concentration-dependent increase of cytokines). The manufacturing process showed impact on the ecotoxicological properties of Cu-based OC (EC50 algae <6.5 to 68 % of the soluble

fraction). The following characteristics were identified as key parameters for the assessment: powder particle size (mean diameter 4.24–175.4 μm) and airborne size distribution (PM10 fraction 8–62% in PM100), dustiness (201–1370 PM100 μg/m³), chemical composition (Mn, Fe, Cu) and manufacturing process. This multidisciplinary study demonstrates the relevance of the SbD approach to assess and manage HSE risks at an early stage of OC development for future energy production.

- **Keywords:** Safe by design; Oxygen carrier; Chemical looping combustion; Exposure; Toxicity – risk assessment

Yang Xiao, Xi Meng, Lan Yin, Qing-Wei Li, Chi-Min Shu, Yuan Tian. *Influence of element composition and microcrystalline structure on thermal properties of bituminous coal under nitrogen atmosphere*. Pages 846-856.

To explore the main influencing factors of atomic ratio (O/C, N/C, and H/C) as well as microcrystalline structure (d002, La, Lc, and Mc) on thermal properties (specific heat capacity, thermal conductivity, and thermal diffusivity) at certain temperatures within 30.0–300.0 °C, three coal samples were collected from coal mines of Dafosi, Yangjiaping, and Hujiahe in Binchang coalfield, Shaanxi Province, PR China. Thermal properties of coal samples were determined by laser-flash apparatus in nitrogen atmosphere. After temperature treated at 30.0, 60.0, 90.0, …, 300.0 °C in nitrogen atmosphere, the atomic ratio and microcrystalline structure of samples were measured by proximate analyser and X-ray diffractometer. The results indicated that with an increment in the temperature, the value of H/C for three coal samples diminished slightly and then promptly, whereas O/C diminished slightly and then increased before 120.0 °C, as well as finally increasing, and the N/C had no obvious change. Concurrently, the microcrystalline structure of coal samples became more orderly and complete. Furthermore, the TD decreased with temperature, the SHC and TC showed an opposite trend with TD. Based upon grey correlation analysis, the major influencing factors of atomic ratio and microcrystalline structure on thermal property were approached. The results provided insight into the physicochemical properties of the coal of interest for predicting the progress of coal spontaneous combustion.

- **Keywords:** Atomic ratio; Specific heat capacity; Thermal conductivity; Thermal diffusivity; Grey correlation analysis; Coal spontaneous combustion

Benqiang Cen, Rui Yang, Kexun Li, Cuicui Lv, Bolong Liang. *Large capacity and rapid rate of ion removal from synthetic municipal wastewater via CDI using chitosan-based nitrogen-doped porous carbon electrode*. Pages 857-865.

Capacitive deionization (CDI) technology has excelled in water treatment areas such as brackish water desalination, hard water softening and pollution ion removal. However, the poor performance of the electrodes used in CDI cell construction continues to limit its practical application. In this work, we used chitosan mixed with potassium hydroxide (KOH) and simply carbonized to synthesize porous carbon electrode materials (CTS-850) with excellent material and electrochemical performance, and achieve high adsorption capacity and fast adsorption rate in a variety of salt solutions. The material characterization of CTS-850 displayed super large specific surface area (>2300 cm3 g−1), pore volume and excellent nitrogen doping. Electrochemical characterization showed excellent specific capacitance, good conductivity and cycle performance. In CDI experiments, we explored the removal efficiency of electrodes carbonized under different temperatures in single and mixed solution systems, and the CTS-850 electrode had an ultra-high adsorption capacity of 47 mg g-1 and a fast adsorption rate of 6.7 mg g-1 min-1 in 15 mM synthetic municipal wastewater (~1750 mg L-1). In addition, we

discussed the relationship between high adsorption capacity, fast adsorption rate and material properties. Our work is expected to provide guidance for the synthesis of higher performance CDI electrode materials.

- **Keywords:** Capacitive deionization; Chitosan; Porous carbon; Nitrogen doping; Electrosorption

Tao Zeng, Guohua Chen, Genserik Reniers, Yunfeng Yang. *Methodology for quantitative risk analysis of domino effects triggered by flood*. Pages 866-877.

Flood events impose great distress on chemical industrial areas, since they may cause Natech accidents involving multiple units. Furthermore, escalation vectors exerted by major accidents can trigger knock-on events, so-called domino effects, causing very severe consequences. In the present study, a methodology is proposed to include domino effects triggered by floods in a quantitative risk assessment, by addressing the frequency assessment of flood-induced domino scenarios. A comprehensive procedure is developed, combining the fragility model for unit damage due to floods, probability estimation for domino escalation, and combinatorial analysis for overall scenarios. Moreover, the flow interference due to the layout of chemical industrial areas is explored to calculate the damage probability more accurately. The methodology has been demonstrated by a case study, the changes in risk indexes and damage zones due to Natech domino effects are discussed. The results show that the overall risk significantly increases with respect to conventional scenarios when considering flood-induced Natech events and domino effects, evidencing the importance of risk analysis of Natech-related domino effects. Finally, some prevention measures have been proposed for chemical industrial areas to make them more resilient and safer when it comes to floods.

- **Keywords:** Flood; Natech event; Domino effect; Probability; Quantitative risk

Muhammad Babar, Ahmad Mukhtar, Muhammad Mubashir, Sidra Saqib, Sami Ullah, Abul Hassan Ali Quddusi, Mohamad Azmi Bustam, Pau Loke Show. *Development of a novel switched packed bed process for cryogenic CO2 capture from natural gas*. Pages 878-887.

Desublimation-based Carbon dioxide (CO2) removal from the natural gas (NG) in a cryogenic packed bed becomes challenging due to the dry ice formation inside the packed bed. Therefore, the cryogenic packed bed has been used for NG purification only in batch processes. However, to fulfill the energy requirements, it is crucial to develop a continuous process for NG purification, which is difficult for a single cryogenic packed bed. In the current research, a novel cryogenic packed bed system is proposed for continuous capture of desublimation based CO2 capture from natural gas. The process feasibility of the switching concept was proved through dynamic simulation and experimental study on CO2 separation from multi-component NG. It was observed that increasing CO2 content decreases the switching and saturation time of the cryogenic packed bed. The total energy required per packed bed per cycle in the switching system is 133.35. The saturation time for pure CO2 feed, NG sample-1, and NG sample-2 were 300, 500, and 600 s, respectively. An excellent agreement was observed between the results obtained from the experimental results and that obtained through dynamic simulation. A switching time of 200 s was found for a CO2 recovery of more than 98 %. This research work offers scientific data and theoretical support for the industrial application of switched cryogenic packed bed setup in CO2 capture from natural gas in the future. Moreover, in the current research work, scale-up study, and automatic control system for the switched packed bed are recommended for the future.

- **Keywords:** Natural gas; Carbon dioxide; Aspen HYSYS; Cryogenic packed bed; Gas separation

Jianmin Fu, Guoming Chen, Xiaoyun Zheng, Qihang Gao, Shenxin Qiu, Zhiqian Xu. *Experimental and numerical studies of insulating layers effect on liquid pipelines leakage in chemical plants*. Pages 888-899.

Study the effect of the insulating layers on the liquid pipeline leakages and determining the leakage profile calculation model is critical and basic for the leakage-associated fire and explosion risk assessments for the chemical process industry. This research carried out a series of experiments, with an attempt to explore the leakage process of insulated pipeline. The experiments display that the leakage is dynamic, which is divided into three stages: initial, transitional and stable period. During the stable period, both the leak rate and pressure of insulated pipeline responding to work condition are different from those of naked pipeline. Then a fundamental formula is derived from the experimental data which is applicable for leakage calculation with insulating layers. Besides, sensitive factors that affect the leak volume are analyzed, among which the thickness of insulating layer is the most influential one. The research has designed a CFD model to reveal the dynamic leakage process in insulating layers and verify the effectiveness and accuracy of experiments. The result of this paper could improve risk assessment preciseness of liquid pipeline leakage.

- **Keywords:** Process safety; Risk assessment; Liquid pipeline leakage; Leak rate; Insulating layer; CFD simulation

Kim Hoong Ng, Siaw Ching Liew, Shaoliang Zhang. *Thermodynamic analysis of CaS production from various Ca-based precursors: A prequel to SO2 reduction mediated by CaS/CaSO4 redox agents*. Pages 900-911.

The competency of CaS in reducing SO2 into pure sulphur was well-validated in past research. However, all pertinent past works monotonically derived CaS from CaSO4 or CaSO4-based materials while overlooking the potential of other Ca-materials in reducing SO2. Current study closes such research gap by assessing the theoretical feasibilities of converting CaCO3, Ca(OH)2 and CaO into CaS via minimization of Gibbs energy. Significantly, two different synthesis paths, namely solid-solid and gas-solid reaction, were conceptualized and assessed herein. In solid-solid synthesis, the formation of CaS is accomplishable in S8-sulphidization of Ca(OH)2 and CaO, with the former one attained lower CaS yield due to low equilibrium conversion. Whereas, in gas-solid operation, H2S appeared to be the strongest sulphidizing agent, with the potential of attaining 100% CaS yield from all three Ca-based precursors, followed by S2 (75 % CaS yield) and SO2 (25 %) under appropriate condition. Auspicious CaS formations are commonly attained at low temperature operation, typically < 1218.15 K for all Ca-precursors. As temperature surpasses 1218.15 K, CaS formation was pronouncedly suppressed, bestowed to the unfavourable thermodynamic restriction. Significantly, the findings in current study revealed the thermodynamic hurdles in synthesizing CaS from different Ca-species, concurrently propagating CaS-mediated SO2 reduction in future studies.

- **Keywords:** CaS formation; Thermodynamic assessment; CaS-facilitated SO2 reduction; SO2 treatment

Vigneswaran V.S., Ganesh Kumar P., Jeyachandran J., Britto Sahayaraj S., Kumaresan G. *Usage of solar greenhouse evaporator to enhance dehydration and potable water extraction from tannery effluent*. Pages 912-923.

The main objective of the present work is to treat tannery effluent with a total dissolved content of 150 g/L using solar energy by humidification and dehumidification process using a roof even type greenhouse evaporator. This system not only helps to effectively treat the tannery effluent by increasing its total dissolved solids content to 350 g/L but

also helps to generate potable water from tannery effluent by using solar energy. In this study, the performance of the effluent was tested in six different modes. It was found that the tannery effluent total dissolved solids content increased to 350 g/L in just 2.5 days when the greenhouse evaporator was operated in Mode 6 which is the shortest duration when compared to other modes of operation. The specific fuel consumption of the roof even type greenhouse system to treat tannery effluent is 22.55 kW h/ m3 which is 8.3 % of the energy consumed by the zero liquid discharge plant. Meanwhile, the land area required to dehydrate 1 m3 of tannery effluent got decreased by 43 % when the roof even type greenhouse evaporator was used.

- **Keywords:** Greenhouse dryer; Tannery effluent; Humidification; Dehumidification; Evaporation rate

Mikel Orive, Marta Cebrián, Javier Amayra, Jaime Zufía, Carlos Bald. *Techno-economic assessment of a biorefinery plant for extracted olive pomace valorization*. Pages 924-931.

This study reports on a new integrated valorization alternative for extracted olive pomace (EOP) by recovering polyphenols as high-value compounds and the subsequent anaerobic digestion of the remaining dephenolized fraction for energy production. The average polyphenol extraction rate was 22.10 kg GAE t^{-1} EOP and the subsequent optimum methane production from the remaining dephenolized fraction (278 L CH_4 kg VS^{-1} d^{-1}) occurred at organic loading rate (OLR) 2.48 g VS L^{-1} d^{-1} and 24 d hydraulic retention time (HRT). The study also reports on the preliminary economic feasibility study and the sensitivity analysis to valorize 1,500 t EOP y^{-1} under biorefinery concept. The calculated net present value (NPV) and internal return rate (IRR) were €1,996,856 and 58 %, respectively. The sensitivity analysis concluded that the minimum sales volume of hydroxytyrosol (HT) extract and the sale price per mass are by far the most significant factors that might influence the overall economic feasibility of the proposed EOP valorization plant.

- **Keywords:** Biorefineries; Polyphenols; Biogas; Economic assessment; Sensitivity analysis

Astrid Barona, Adrián Malo, Ana Elías, Naiara Rojo, Arrate Santaolalla, Gorka Gallastegui. *A feasibility study of the installation of a modular bioreactor inside a chemical scrubber at a wastewater treatment plant*. Pages 932-941.

Chemical scrubbing and biofiltration are well-established technologies for treating contaminated pollutants generated at wastewater treatment plants (WWTPs). Nevertheless, the growing need to reduce the ecological footprint of abatement technologies without affecting process efficiency is prioritizing biological alternatives. This study deals with the challenge of designing a structure for converting a chemical scrubber currently operating at a WWTP with a capacity of 6400 population equivalent (PE) into a modular bioreactor without any actual modification of the scrubber´s structure. The inside of the reactor was divided into three levels or platforms for holding the biomaterial, and the corresponding parts were manufactured in PVC, with the exceptions of the screws and cross bracing. The study of the parts' stress and strain limits revealed that the slats and half-rings should be reinforced with ribs, and the optimal rib height was studied on a case-by-case basis. It was also concluded that the base legs could hold the weight of 80 cm height biomaterial bed onto each of the three platforms. Based on previous studies, the converted biofilter with an inlet flow rate of 1150 m3/h could render simultaneous removal efficiencies greater than 90 % for H_2S and NH_3. Regarding the viability study, the annual savings from the elimination of chemical consumption were around 9.7 % of the total investment cost. One of the main

strengths of replacing the scrubber with a biofilter was the improvement in sustainable performance and health and safety, reducing both risk and the budget for prevention.

- **Keywords:** Chemical scrubber; Modular biofilter; Odour pollution abatement; Wastewater treatment plants; Feasibility

Sumona Show, Saumyajeet Mukherjee, Moirangthem Sarda Devi, Bisheswar Karmakar, Gopinath Halder. *Linear and non-linear analysis of Ibuprofen riddance efficacy by Terminalia catappa active biochar: Equilibrium, kinetics, safe disposal, reusability and cost estimation*. Pages 942-964.

The presented work assesses the sorptive efficacy of acid and base activated biochar engineered from bio-waste tropical almond shells for eradicating Ibuprofen (IBP) from aqueous media. Adsorbents were characterized by proximate, FTIR and SEM analyses. Impact of various parameters like IBP concentration, pH, agitation speed, sorbent dose, interaction time and temperature on sorptive expulsion were studied using experiments focussed on elucidating optimal conditions. Batch sorption and optimization studies using central composite design revealed that highest IBP removal of 92.46 % and 92.8 % respectively using TABAB were attainable with a 15 mg/L initial IBP solution containing 3.33 g/L adsorbent dose at pH 2 under 35 °C within 6 h at 150 rpm. Performance of IBP sorptive removal was verified by linearized and non-linearized approaches on kinetic and isotherm models. Langmuir isotherm model was the best fit with maximum adsorption capacities of 2.794 mg/g and 8.77 mg/g under acid activation for linear and non-linear analyses respectively while noted adsorption capacities under base activation were 2.914 mg/g and 9.52 mg/g for linear and non-linear analyses respectively. A pseudo second order kinetic model best fits the findings from both analyses. Thermodynamic studies suggested a randomness with exothermic nature of the viable removal process. With both biochar showing effective reusability for 4–5 cycles, estimated preparation costs were an approximated 0.24 INR for treating 1 L of solution with optimal IBP concentration. Consequently, modified adsorbents obtained from tropical almond shell char can be used as cost-effective adsorbents for IBP removal.

- **Keywords:** Ibuprofen; Tropical almond shells; Linear; Non-linear; Isotherm; Kinetics; Thermodynamics; Cost estimation

Xiaoqing Li, Yuze Fan, Renqiang Liu, Ying Xu, Xiaoyan Liu. *Numerical investigation of oil droplets motion in water using LBM*. Pages 965-971.

The safe transportation of waxy crude oil is a key in the field of pipeline gathering and transportation. The motion characteristics of an oil droplet in water for safe transportation are numerically analyzed in this paper. The mathematical model of oil-water two-phase flow under pipeline transportation conditions is established and solved by LBM (lattice Boltzmann method). The influences of interfacial tension, contact angle and the viscosity of oil on the flow characteristics of oil droplets, such as deformation and fracture were investigated after validating the model. The results indicate that deformation of the oil droplet is mainly determined by interfacial tension and oil viscosity, while the affect of contact angle is not substantial. With the increase of interfacial tension and the viscosity of oil, the maximum deformation of droplets before fracture decreases. It is found that the contact angle has a significant effect on the number of broken droplets and the shape of the oil droplets. While the critical time of the initial fracture is mainly defined by the viscosity. In addition, the interfacial tension also has a slight influence on the critical time of the initial fracture.

- **Keywords:** Multiphase flow; Oil-water; Numerical investigation; LBM

Zainab Al Ani, Ashish M. Gujarathi, G. Reza Vakili-Nezhaad. *Simultaneous energy and environment-based optimization and retrofit of TEG dehydration process: An industrial case study*. Pages 972-984.

Carbon dioxide emissions (CO2) during the dehydration process of natural gas are of important concerns as this gas negatively affects the climate and environment in general. Dehydration process also encounters many heating, cooling and pumping units, which leads to high energy consumption. Reducing these emissions along with minimizing the utilized energy while keeping the high production is a complex problem that can be solved by multi objective optimization (MOO). This study focuses on minimizing CO2 emissions, energy consumption (ENG) along with water content in the gas (WT). This means that the performance of the plant is improved from operational, environmental and energy point of view. The process is simulated with ProMax 4.0 and approved to be valid with the real plant data. Non-dominated sorting genetic algorithm (NSGA-II) was used for attaining the Pareto fronts for the decided MOO cases. The affecting decision variables and limitations are decided based on the capacity of the plant and industrial practice. Two bi-objective cases and a tri-objective case are considered, which are; minimizing CO2 emissions and WT (case 1), minimizing ENG and WT (case 2) and minimizing WT, ENG and CO2 emissions simultaneously (case 3). An attempt to retrofit the current process is also proposed and the cases are carried out with the modified process. Results showed noticeable improvements and enhancements in the given process.

- **Keywords:** Dehydration; Retrofitting; Evolutionary algorithms; Energy; Global warming; CO2 emissions; Pareto ranking

Jianjun Cai, Wenheng Zheng, Ming Luo, Xingying Tang. *Gasification of biomass waste in the moving-grate gasifier with the addition of all air into the oxidizing stage: Experimental and numerical investigation*. Pages 985-992.

The moving-grate gasifier has some significant advantages over other types of gasifiers. This is because the residue time of the biomass waste in a moving-grate gasifier can be controlled in a suitable range for optimizing thermochemical conversion efficiency. In addition, the moving-grate gasifier is more suitable for having biomass waste fed into it. This study investigated the gasification behaviours of biomass waste in the moving-grate gasifier with the addition of all air being done in the oxidizing stage. In the experimental samples, the average cold gas efficiency in the moving-grate gasifier was 64.79 %, and the high temperature region in the moving-grate gasifier was converted to the pyrolysis. The lower heating value (LHV) of flue gas in the large-scale moving-grate gasifier was 5570 kJ/m3 and the cold gas efficiency was 67.50 %. From this observation, it can be concluded that the gasification performance of the large-scale moving-grate gasifier was better than that of the small-scale.

- **Keywords:** Biomass waste; Gasification; Moving-grate gasifier; Primary air

Qian Sun, Deli Lin, Majid Khayatnezhad, Mohammad Taghavi. *Investigation of phosphoric acid fuel cell, linear Fresnel solar reflector and Organic Rankine Cycle polygeneration energy system in different climatic conditions*. Pages 993-1008.

It has been proven that the future of energy demands for human society is related to clean energy sources such as solar energy. On the other hand, fuel cell technology converts the chemical energy of a fuel into electrical energy. Meanwhile, the polygeneration system based on (semi) renewable energy can be a viable alternative to conventional fuel-based systems. However, examining their performance for widespread

implementation requires further and powerful studies. The aim of the present work is to evaluate the performance of the polygeneration energy system to produce electricity, heat, hydrogen and cool. The novel hybrid power system consists of the 10 kWel phosphoric acid fuel cell, linear Fresnel solar reflector (LFR), Organic Rankine Cycle (ORC) and Stirling engine (SE). In the novel energy conversion process proposed, the fuel cell generates electricity and heat, and its waste heat is used to generate additional electricity in the SE. The fuel and oxidant required by the fuel cell are supplied by an electrolyzer that is powered by an ORC system. A solar thermal collector provides the duty required by the evaporator of ORC system. The effect of key parameters such as current density, solar radiation and flow rate of hydrogen on the system energy and exergy performance is also investigated. To evaluate the performance of the LFR system the climatic conditions of Tehran (in Iran) and Beijing (in China) are considered. Results revealed that, the SE and ORC system separately generates 1.48 and 26.54 kW of electricity, respectively. Furthermore, the electrolyzer consumes 23.36 kW of electric power and 3.64 kW of cooling is produced by the chiller. In addition, the energy efficiency and total exergy destruction of the proposed system are 71.32 % and 57.94 kW, respectively.

- **Keywords:** Phosphoric acid fuel cell; Linear Fresnel reflector; Organic Rankine Cycle; Stirling engine; Hybrid system; Parametric study

Chen Wang, Long Ding, Huaxian Wan, Jie Ji, Yonglong Huang. *Experimental study of flame morphology and size model of a horizontal jet flame impinging a wall*. Pages 1009-1017.

The production and transportation processes of gas fuel may be faced with a safety challenge in the form of a jet fire from pipeline leakage. In actual accidents, sometimes some obstacles may appear in the path of the horizontal jet fire development leading to impingement. The spread mechanism of such a flame is complex due to the coupling relation of the wall resistance force, buoyancy force and initial momentum. Experiments were conducted to study a horizontal jet flame impinging a wall as a function of fuel initial velocity and nozzle-wall spacing. Results show the transient development of flame morphology and spread mechanism of the steady flame. The upward buoyancy force of the horizontal jet flame gradually increases with the fuel as it moves further away until flame impinges the wall. From the side view, flame morphologies include the flame impinging the wall (up-down spread and up spread stages) and flame not impinging the wall (free spread stage). A counterclockwise flame vortex occurs due to the competition between the upward buoyancy force and downward momentum below the nozzle projection point. From the front view, the flame morphology changes from "U" morphology to "O" morphology. By combining the knowledge of the jet fluid, momentum conservation principle and Newton's second law, a flame size model of the horizontal jet flame impinging the wall is proposed.

- **Keywords:** Horizontal jet flame; Impinging the wall; Flame morphology; Flame size model; Production and transportation processes

Dishit P. Ghumra, Chandrodai Agarkoti, Parag R. Gogate. *Improvements in effluent treatment technologies in Common Effluent Treatment Plants (CETPs): Review and recent advances*. Pages 1018-1051.

Common Effluent Treatment Plants (CETP) are intended for effective treatment of effluent discharged from industrial clusters aiming to support the small/medium scale industries that are deprived of enough resources and technological ability to treat their effluent individually. The present review discusses various processing steps in a typical CETP and their design considerations. The various drawbacks of existing CETPs have been discussed with the need for requirement of novel treatment techniques for their reformation. The different novel approaches discussed include improved coagulation-

flocculation, advanced oxidation processes like electrochemical oxidation, cavitation, Fenton, ozonation and photocatalysis. Additionally, possible improvements in the biological treatment methods have also been discussed. Possible applications of bioremediation methods like phytoremediation, constructed wetlands, microbial fuel cells, use of fungi and algae have been highlighted. Membrane technologies and physicochemical treatments coupling with biological oxidation have also been described. For each method, mechanism involved, recent advances and possible recommendations for operating conditions have been provided. The economic aspects of the effluent treatment have also been discussed to aid the transformation of existing CETPs. Overall, the review clearly brings out the important novel techniques having potential to be applied in the existing CETPs and modifications in the existing approaches for their performance enhancement.

- **Keywords:** Advanced oxidation processes (AOPs); Common Effluent Treatment Plant (CETP); Bioremediation; Membrane technologies; Hybrid treatment processes; Intensification

Gamal B. Abdelaziz, Emad M.S. El-Said, Ahmed G. Bedair, Swellam W. Sharshir, A.E. Kabeel, Ashraf Mimi Elsaid. *Experimental study of activated carbon as a porous absorber in solar desalination with environmental, exergy, and economic analysis*. Pages 1052-1065.

In this study, an experimental investigation is carried out to assess solar still (SS) performance with a porous absorber made from activated carbon tubes (RACT) with four various arrangements based on energy, exergy, economic, environmental, exergoeconomic (EXC), enviroeconomic (ENC), exergoenvironmental (EXE), and exergoenviroeconomic (EEC) points of view. Activated Carbon (AC) is utilized as a black porous absorber. The conventional SS without porous material (SS-C) is also experimentally studied for comparison. The performance of the five models is tested under practical operating conditions. The results indicated that solar still with horizontal staggered half capacity (SS-HSC) achieved high performance depending on energy, exergy, cost, EXC, EXE, and EEC. The daily water yield of SS-HSC is about 5850 ml/m2 with about 38.82 % decrement cost, compared to SS-C. The energy and exergy efficiencies of SS-C are augmented by about 94.14 % and 164.29 % with operating mode SS-HSC respectively. The CO2 net emissions mitigated per year based on energy and exergy concepts for SS-HSC are 31.11 and 1.19 tons respectively. The ENC parameter and the EXE analysis for SS-HSC are rated by about 451.09 $ and 17.24 $, respectively. The utilizing of RACT gives a positive impact on energy, exergy, economic and environmental performance.

- **Keywords:** Activated carbon tube; Solar distiller; Exergy; Economic; Environment

Haiqing Xu, Liang Guo, Yangguo Zhao, Mengchun Gao, Chunji Jin, Junyuan Ji, Zonglian She. *Accelerating phosphorus release from waste activated sludge by nitrilotriacetic acid addition during anaerobic fermentation process and struvite recovery*. Pages 1066-1076.

Phosphorus (P) recovery from waste activated sludge (WAS) could achieve sustainable development and reduce environmental hazards simultaneously. The objective of this study was to enhance P release from WAS by nitrilotriacetic acid (NTA) addition and struvite recovery. The maximal P release efficiency reached 90.3 % from WAS at the dose of 25.0 mM NTA after anaerobic fermentation 12 h. The NTA addition promoted nonapatite inorganic phosphorus (NAIP) and apatite phosphorus (AP) release from WAS while it had a negative effect on organic phosphorus (OP) release. The NTA was beneficial for the protein release from WAS, but it inhibited the release of NH4+-N. By means of struvite precipitation, the PO43−-P and NH4+-N recovery rates at optimal

initial pH = 9 of the fermentation supernatant reached 92.9 % and 51.5 %, respectively. Meanwhile, the purity and yield of the produced struvite were 85.8 % and 174.0 mg/g SS (per gram of dry sludge) determined by elemental analysis, respectively. The levels of heavy metals in struvite products were below the permissible limits of Cultivated Land Application Standard. Therefore, the results of this study enriched the P recovery path from WAS to guide the application.

- **Keywords:** Waste activated sludge; Nitrilotriacetic acid addition; Anaerobic fermentation; Struvite recovery

Hasan Arslanoğlu, Fikret Tümen. *Potassium struvite (slow release fertilizer) and activated carbon production: Resource recovery from vinasse and grape marc organic waste using thermal processing*. Pages 1077-1087.

This study investigated the production conditions of a potassium magnesium phosphate fertilizer with vinasse (a by-product of the sugar or ethanol industry) and grape marc (a by-product of the wine-making industry). A mixture of vinasse and grape marc was subjected to pyrolysis under a nitrogen gas atmosphere, and water was used to extract potassium from the end product. Potassium magnesium phosphate (potassium-struvite, KMgPO4.6H2O), a slow-release fertilizer compound, was obtained from the extract with potassium to explore process conditions and product characteristics. Producing fertilizer products from residual materials is of paramount significance for conserving natural resources. The mixture was pyrolyzed, allowing us to remove potassium from the complex matrix of concentrated vinasse to a clear and high alkaline solution. The residual carbon was activated by decomposing (pyrolysis) and treating the residue and then washing it with water. The extract had high alkalinity, suggesting that the potassium in the mixture resulted in carbon activation during biomass pyrolysis. Pyrolysis and treatment can be used to produce activated carbon from vinasse. This study also investigated the solubility of vinasse in water and aqueous solutions. K-struvite with 10.67 % K2O was about 2% soluble in water, indicating that the end product was a slow-release fertilizer agent. In conclusion, this process can be used to produce potassium (a slow-release fertilizer) and activated carbon (a by-product) from vinasse for different purposes.

- **Keywords:** Vinasse; Grape marc; Pyrolysis; Potassium-struvite; Slow-release fertilizer; Activated carbon; Circular economy

Ping Wu, Xujie Zhang, Jiajun He, Siwei Lou, Jinfeng Gao. *Locality preserving randomized canonical correlation analysis for real-time nonlinear process monitoring*. Pages 1088-1100.

Hazard identification and analysis is an important step in the process safety assessment/management in the modern process industry. For hazard identification, real-time monitoring of process operations plays a critical role to establish required safety measures. In this paper, a novel locality preserving randomized canonical correlation analysis (LPRCCA) method is proposed for real-time nonlinear process monitoring. The basic idea is to map the original data onto a randomized low-dimensional feature space through random Fourier feature map, and then integrate the local geometric structure information to improve data mining performance. On the basis of explicit low-dimensional random Fourier features, the computational cost of the online feature extraction is dramatically reduced. The proposed LPRCCA method is significantly more favorable than kernel-based methods for nonlinear process monitoring. The applicability and effectiveness of the proposed process monitoring scheme are verified through a numerical example and an industrial benchmark of the Tennessee Eastman process (TEP) by the comparisons with other relevant methods.

- **Keywords:** Canonical correlation analysis; Random Fourier feature map; Local geometric structure information; Kernel methods; Real-time process monitoring

Guochun Li, Chuanyu Pan, Yangpeng Liu, Xiaolong Zhu, Xiaomin Ni, Xiangdi Zhao, Guoxin Chen, Xishi Wang. *Evaluation of the effect of water mist on propane/air mixture deflagration: Large-scale test*. Pages 1101-1109.

Oil and gas explosions threaten the process of industrial protection and personal safety, and explosion risk control/reduction has always been an important issue. As a clean and efficient fire-extinguishing agent, water mist has been evaluated via small-scale tests as a potential efficient material for reducing explosion hazards. To deepen the understanding of large-scale explosion mitigation using actual water mist, which is typically used for fire suppression, a series of experimental tests were conducted using a large explosion vessel (with a 1.5 m × 1.5 m section and a 10 m length). Explosion characteristics—flame propagation process and speed, explosion overpressure, and explosion overpressure rise rate—were determined and analyzed based on the measured data obtained using a Phantom high-speed camera, flame sensors, and pressure sensors, respectively. Two different types of water mist nozzles, different constraints of the vessel and set locations of the nozzles, as well as water mist additives were considered. The results indicated that both the characteristics of the water mist spray and the installation locations of the nozzles have significant effects on the explosion mitigation. In addition, it was found that the K2CO3 additive can double the explosion mitigation effect of water mist using nozzle A, however, this effect is weaker than that when using nozzle B without K2CO3. Therefore, the effect of K2CO3 additive on the explosion mitigation is weaker than of the change in the water mist characteristics. These results will be relevant for further understanding the process safety of explosion mitigation using water mist under large-scale conditions and for the optimum safety design of water mist explosion mitigation systems.

- **Keywords:** Explosion characteristic; Large-scale deflagration; Explosion mitigation; Safety; Water mist; Additive

Xudong Zhen, Zhi Tian, Yang Wang, Daming Liu, Xiaoyan Li. *A model to determine the effects of low proportion of hydrogen and the flame kernel radius on combustion and emission performance of direct injection spark ignition engine*. Pages 1110-1124.

The only product of hydrogen combustion is water, so it is very clean. In this paper, the effects of low hydrogen content and FKR on the performance of the GDI engine are mainly studied. The simulation results show that adding less than 3% hydrogen in the GDI engine can improve the BP and BT of the engine under typical urban conditions such as 1500 rpm and 2000 rpm. As the hydrogen volume fraction and the FKR increase, the LFS of the mixture increases, resulting in a shorter ignition delay, combustion delay, and 10–90 % MFB. However, an increase in FKR results in a decrease in the BP and BT. In terms of fuel economy, the BSFC decreases as the hydrogen content increases, but as FKR increases, the BSFC increases. In terms of emissions, the proportion of hydrogen increases, HC and NOx emissions increase, and CO and CO2 emissions decrease. Therefore, adding hydrogen to the GDI engine while adjusting the FKR can improve the dynamic performance of the engine and reduce CO and CO2 exhaust emissions.

- **Keywords:** Hydrogen; Flame kernel radius; Combustion and emissions; GDI

Zijun Li, Yu Xu, Huasen Liu, Xiaowei Zhai, Shuqi Zhao, Zhijin Yu. *Numerical analysis on the potential danger zone of compound hazard in gob under mining condition*. Pages 1125-1134.

For years, the methane (CH4) explosion accidents initiated by spontaneous coal combustion took hundreds of lives and destroyed billion possessions in the process of mining. This work developed a fully coupled model involving complex interactions between oxygen transport and airflow, coal spontaneous combustion, CH4 emission and migration. The aim was to analyze the potential danger zone of combined hazard posed by spontaneous coal combustion and CH4 build-up in mine. Unlike traditional fixed mesh that the working face and gob are fixedness, a moving mesh method was incorporated in the model to perform the dynamic gob as the advancing of working face. The moving mesh is modified by the algorithm of Laplace smoothing to avoid mesh distortion and advance the mesh quality. The dynamic distribution characteristics of the porosity, oxygen and CH4 concentration in the gob under mining condition were determined using numerical simulations. According to the theory of the compound hazard, the highest degree of compound hazard zone is identified. The results show that the zone representing the highest degree of compound hazard is located mainly in the middle of the strike directions of the working face, as well as a small part of it on the return airway side and closer to the working face. It was analyzed that the variations in location of potential danger zone under different ventilation flux, the advancing rate of the working face and the attenuation coefficient of CH4 release. Meanwhile, the governance methods for the compound hazard in the gob have been further discussed. This research can provide a guidance on the prediction and control of compound hazard represented by spontaneous coal combustion and methane emission, thus ensuring the safety production.

- **Keywords:** Compound hazard; Potential danger zone; Moving mesh; Spontaneous coal combustion; CH4 distribution; Numerical simulation

Muhammad Zahoor, Sabzoi Nizamuddin, Srinivasan Madapusi, Filippo Giustozzi. *Recycling asphalt using waste bio-oil: A review of the production processes, properties and future perspectives*. Pages 1135-1159.

Roads play a crucial role in the economic development of nations; reconstruction, resurfacing, or rehabilitation of the current roads result in the milling of approximately 120 million tons of asphalt pavement every year. Due to the significant volume of resources involved, road agencies constantly trade-off among economic, performance and environmental challenges to maintain and build road assets. To address these challenges – such as reducing the dependency on non-renewable petroleum-based products and minimising waste and landfills – recycling of end of life road material through various organic binders has been evaluated. Bio-oil, obtained through recycling of different sources, contains lower molecular weight components that resemble fractions of the virgin asphalt binder used to make roads. This review article focuses on the recycling of bio-oil and its utilization in asphalt binders – as an alternative, extender, modifier and rejuvenator – and asphalt mixes. This review paper provides information on the production methodology used to produce bio-oil from various types of biomass, along with upgradation techniques adopted to upgrade the bio-oil before its addition into bitumen. The chemical and physical properties of bio-oils vary for each type of biomass. The production methodology to produce bio-binder from bio-oil is also specified. Simultaneously, the effect of bio-oil on the mechanical, rheological and chemical properties are compared with those of conventional bitumen. It is concluded that the performance of bio-binder varies with the type of bio-oil used for the modification, generally improving the intermediate and low-temperature viscoelastic behaviour but reducing the high-temperature performance. This review article provides a sketch of favourable and harmful aspects associated with the utilization of bio-oil to form bio-binders.

- **Keywords:** Bio-oils; Reclaimed asphalt pavement (RAP); Rejuvenator; Recycling; Bio-asphalt; Organic based binder

Yu Zhang, Zehua Ji, Yuansheng Pei. *Nutrient removal and microbial community structure in an artificial-natural coupled wetland system*. Pages 1160-1170.

An artificial-natural coupled wetland was constructed at an estuary between an upstream river and a downstream lake to transport river water and reduce nutrient input load into a grass-type shallow lake. The removal efficiencies of chemical oxygen demand (COD) and total nitrogen (TN) were as high as 43 % and 83 %, respectively. Their concentrations were reduced to 30.98 mg/L and 0.79 mg/L, respectively. The lotus pond had high microbial diversity and was key for water purification. It contributed 19 % and 49 % of the removal efficiencies of COD and TN, respectively. Most of the dominant microorganism in wetland were related to the transformation of C and N. Bacterial phyla containing phototrophic members accounted for three-quarters of the microorganisms and significantly contributed to bioactivity. Phylum Proteobacteria, the most abundant microbial species, were involved in both N and C cycling because of the metabolic versatility. The denitrification of the wetland depended on the classes Gammaproteobacteria, Deltaproteobacteria, Bacteroidia and Anaerolineae. Bacteria of the phyla Chloroflexi, Actinobacteria, Firmicutes, Spirochaetes, Bacteroidetes and class Alphaproteobacteria contributed to hydrocarbon mineralization and carbonate decomposition to promote C cycling. Therefore, this study provides insights to develop effective methods for reducing the risks of lake eutrophication and protecting the water ecological health.

- **Keywords:** Artificial-natural coupled wetland; Nutrient load; Denitrification; Microbial community; Proteobacteria

Mohammed El Ibrahimi, Ismail Khay, Anas El Maakoul, Mohamed Bakhouya. *Food waste treatment through anaerobic co-digestion: Effects of mixing intensity on the thermohydraulic performance and methane production of a liquid recirculation digester.* Pages 1171-1184.

This paper investigates the thermohydraulic performance and methane production of a Liquid recirculation Mesophilic Digester with Submerged solid waste (LMDS) under different mixing strategies. A combination of food waste and cow dung was used as a substrate in the co-digestion experiments. After 24 days of digestion, we reported a higher specific methane yield (301.84 Nm3 CH4 tvs−1) when gentle mixing was adopted, compared to intense mixing (221.32 Nm3 CH4 tvs−1). As for the unmixed co-digestion, it produced the lowest methane yield (112.88 Nm3 CH4 tvs−1). Furthermore, the thermal study showed that the gentle mixing caused less heat loss from the LMDS (20.90 kWh) compared to the intense mixing (40.21 kWh). Moreover, CFD results showed that intense mixing caused a higher pumping energy consumption (through increasing pressure drop) without inducing a significant improvement in the mixing inside the LMDS. Additionally, the liquid flow fields, force distribution, and percolation of the submerged waste were qualitatively evaluated for the considered mixing strategies. Based on these findings, we presented several recommendations aimed at reducing thermal and hydraulic energy losses while guaranteeing optimal methane production in LMDS digesters.

- **Keywords:** Anaerobic digestion; CFD analysis; Heating performance; Hydraulic evaluation; Leachate recirculation; Methane production

Sijie Ge, Yiling Xu, Sujing Wang, Qiang Xu, Thomas Ho. *A win-win strategy for simultaneous air-quality benign and profitable emission reduction during chemical plant shutdown operations*. Pages 1185-1192.

Although the flaring system is designed for the safety operation in chemical plants, the intensive flaring will cause not only tremendous raw material loss, but also large amounts of VOCs and NOx, which could escalate regional ozone formation and elevation under the solar radiation. Thus, it will be a win-win situation to preform air-quality conscious flare minimization (FM) for chemical plants, so that both environmental and industrial sustainability could be promoted. In this study, a systematic multi-scale methodology has been established to identify and demonstrate the win-win strategy for simultaneous air-quality benign and profitable emission reduction during chemical plant shutdown (CPS) operations. The major contribution of this study is that process-level dynamic simulations via Aspen Plus Dynamics have been seamlessly integrated with the regional-level air-quality modeling via CAMx to simultaneously accomplish both flare source savings and ozone impact minimization during the CPS operation. Case studies have indicated that the base case of CPS without FM could have a serious effect on the air-quality (1.6 ppb 8-h ozone observed). However, the improved case of CPS based on FM would significantly reduce such an ozone impact (only 0.1 ppb 8-h ozone observed); meanwhile the flare source and CO2 emission reductions, as well as the plant economic savings are respectively 165.2 tons, 479.1 tons, and US$133,945.6.

- **Keywords:** Ozone pollution control; Chemical plant shutdown; Emission reduction; Dynamic simulation; Multi-scale modeling

Lianhua Cheng, Huimin Guo, Haifei Lin. *Evolutionary model of coal mine safety system based on multi-agent modeling*. Pages 1193-1200.

To investigate the evolutionary mechanisms of coal mine safety systems, and to improve the level of system safety, this paper introduces a new method of assessing and managing the system safety of coal mines. A multi-agent modeling and simulation method is used to construct a dynamic evolutionary model of a coal mine safety system based on complex adaptive system theory. The NetLogo platform is used to design experiments that dynamically simulate the interactions between leaders, managers, and operators under different conditions, and to assess their impact on system safety. The results reveal that the influence of each agent on system safety is different, and safety leadership, safety management, behavioral safety, and environmental suitability all directly or indirectly affect system safety. Among these factors, the safety management level and operators' behavioral safety level exert the strongest influence on system safety. Therefore, in the specific implementation of safety management, coal mine enterprises should adjust and control these attributes to reduce accidents and improve system safety.

- **Keywords:** Coal mine; Enterprise safety system; Complex adaptive system; Agent-based modeling; NetLogo; Simulation

Fei Luo, Lile He, Ning He. *Simulation and experimental study of working characteristics of an improved bioreactor for degrading oily sludge*. Pages 1201-1208.

The degradation characteristics of oily sludge in the bioreactor were studied by using Euler-multiphase flow method, in which the gas-liquid two-phase and gas-liquid-solid three-phase flow field dynamics model was established. The working characteristics of the conventional bioreactor and the proposed new bioreactor were simulated via FLUENT software respectively, and the distribution of bubble diameter and the accumulation and dispersion phenomenon of the oily sludge particles were studied. The experimental results showed that compared with the conventional bioreactor, the proposed one can significantly improve the degradation efficiency of oily sludge and greatly reduce energy consumption.

- **Keywords:** Bioreactor; Oily sludge; Euler-multiphase flow; Degradation characteristics

Jun Zhao, Ling Ma, Mohamed E. Zayed, Ammar H. Elsheikh, Wenjia Li, Qi Yan, Jiachen Wang. *Industrial reheating furnaces: A review of energy efficiency assessments, waste heat recovery potentials, heating process characteristics and perspectives for steel industry*. Pages 1209-1228.

In the world's competitive industrial market, the development of existing manufacturing equipment's such as industrial reheating furnaces (IRFs) increases profitability in terms of higher production, higher quality, and better energy efficiency. In this review, recent progress and current status in IRFs technology have been presented. A special focus has been highlighted on the recent applications and developments of zone modeling and computational fluid dynamic (CFD) simulations in IRFs, paying particular attention to the integration of slap heating processes characteristics, flow and radiative heat transfer analyses, control strategy, and optimization of the furnace. Moreover, the energy efficiency assessment in terms of efficiency models, long-term measurements, and combustion performance improvement techniques (namely, the effect of burner design and oxy-fuel enrichment) for energy saving and thermal efficiency improvement in IRFs is analyzed. Additionally, studies that investigated the use of different waste heat recovery (WHR) systems within IRFs, to evaluate the potential recovery efficiencies and suitability of the IRFs are discussed in details. The reviewed results showed that the energy apportionment model is the most widely used and regarded as an efficient prediction tool for determining the slap energy efficiency of each heating zone in the furnace. Moreover, the Oxy-fuel combustion technique achieved significant improvements in fuel consumption of the IRF, as it fulfilled high energy-saving improvements of 16 %–26.2 %, compared to the air/fuel combustion. In WHR scope, the findings demonstrated that the potential of WHR in IRFs for the steel industry is within the range of high-medium temperature, and significantly improved the furnace overall efficiency and reduced the fuel consumption required in the furnace via the use of waste heat preheaters/units, and recuperative and regenerative burners in IRFs. Noteworthy discussions, important challenges, critical conclusions, and future strategies for each aspect are also discussed as well.

- **Keywords:** Reheating furnaces; Energy efficiency improvement; Waste heat recovery; Zone modeling; CFD; Oxy-fuel combustion; Slap heating process characteristics