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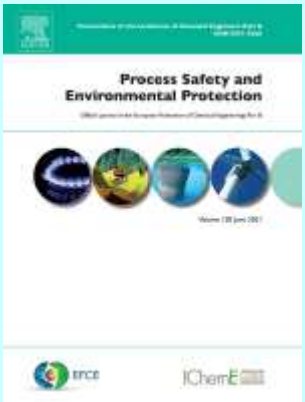

Wenying Wu, Aizhu Wei, Weixing Huang, Peng Zhao, Martin Schmidt, Ulrich Krause, Dejian Wu. *Experimental and theoretical study on the inhibition effect of CO2/N2 blends on the ignition behavior of carbonaceous dust clouds*. Pages 1-10.

Gaseous inhibitors are used in many industries for the explosion prevention of combustible dusts, mitigating the potential hazard to humans, properties and environments. This work experimentally and theoretically studied the inerting effect of gaseous inhibitors on the ignition process of dust clouds in O2/N2/CO2 atmospheres, with an emphasis on the role of the CO2/N2 ratio. 10 different combustible carbonaceous dusts were selected, including grain dust, biomass dust and coal dust. Experimental results showed that the inhibition effect of CO2/N2 is closely related to the ignition mechanism of dust clouds. Specifically, a higher ratio of CO2/N2 yields a stronger inhibition effect on the ignition process of dust samples with relatively low volatile matter contents predominated by heterogeneous ignition. In addition, two novel steady-state ignition mechanism models were developed to interpret the experimental observations. Maxwell-Stefan equations were used to describe the diffusivity in the ternary O2/N2/CO2 gas mixtures. The analytical results were in good agreement with the experimental data of the minimum ignition temperature of dust cloud (MITC) in oxygen-lean atmospheres. The mechanism modelling can be used to estimate the critical ignition temperature of all carbonaceous dust clouds with a wide range of volatile matter content under different inert atmospheres, which will provide a reference for the explosion hazard assessment of dust posed by a hot surface in the process industries.

- **Keywords:** CO2/N2 ratio; Inerting effect; Volatile matter content; MITC; Mechanism model

Lu-Qing Wang, Ting Li, Hong-Hao Ma. *Explosion behaviors of hydrogen-nitrous oxide mixtures at reduced initial pressures*. Pages 11-18.

In this study, we report the explosion characteristics of H2/N2O mixtures at fuel-lean side and stoichiometric condition in a 113 L cylindrical vessel. Experiments were performed at different sub-atmospherical pressures (P0 =10 kPa–40 kPa). Explosion

pressure traces were obtained by a pressure transducer mounted on the wall. Meanwhile, the flame morphology was recorded using schlieren visualization. The maximum explosion pressure (Pmax) and maximum pressure rise rate ((dp/dt)max) were derived and discussed. Results show that two competitive effects (i.e., the adiabatic flame temperature and the molecular number) make the maximum Pmax occurring at φ =0.5—0.6. Linear correlations were found between Pmax and P0. Except the adiabatic flame temperature and flame propagation speed, the flame instability was found to participate in dominating the maximum pressure rise rate. For increased initial pressure, the equivalence ratio of the maximum (dp/dt)max switches to the lean side due to the enhanced flame instability. Depending on different equivalence ratios, both linear and quadratic correlations were found between (dp/dt)max and P0.

- **Keywords:** Hydrogen explosion; Nitrous oxide; Maximum explosion pressure; Flame instability

Peter Schmitz, Genserik Reniers, Paul Swuste. *Predicting major hazard accidents by monitoring their barrier systems: A validation in retrospective*. Pages 19-28.

OCI Nitrogen, one of Europe's largest fertilizer producers, is investigating the extent to which it is possible to take targeted measures at an early stage and stop the development of major hazard accident processes. An innovative model has been developed and recently explained and elaborated in a number of publications. This current paper contains a validation of the model by looking at the BP Texas City incident in 2005. The bowtie metaphor is used to visually present the BP Texas City refinery incident, showing the barrier system from different perspectives. Not only is the barrier system looked at from its trustworthiness on the day of the incident but also from the perspective of the control room operator, and from a design to current standards of best practice. The risk reductions of these different views are calculated and compared to their original design. In addition, evidence and findings from the investigations have been categorized as flaws and allocated to nine organizational factors. These flaws may affect the barrier system's quality or trustworthiness, or may act as 'accident pathogens' (see also Reason, 1990) creating latent, dangerous conditions. This paper sheds new light on the monitoring of accident processes and the barrier management to control them, and demonstrates that the BP Texas City refinery incident could have been foreseen using preventive barrier indicators and monitoring organizational factors.

- **Keywords:** Process safety; Bowtie; Indicator; Organizational factor; Management delivery system

Ji Hun Bang, Christian Ariane Santos, Young Min Jo. *Energy efficient treatment of indoor volatile organic compounds using a serial dielectric barrier discharge reactor*. Pages 29-36.

Volatile organic compounds (VOCs) generated in urban workplaces have been considered as significant air pollutants both indoors and outdoors. In order to reduce those harmful VOCs from urban emission sources, a non-thermal plasma reactor equipped with dielectric barrier discharge (DBD) using alternating current (AC) was investigated with a focus on process design including recirculation. Decomposition efficiency of low concentration VOCs was evaluated in terms of energy yield and conversion selectivity. At 20 ppm, the highest decomposition efficiency (97.3 %) was achieved in the treatment of n-hexane, followed by toluene at 96.6 %, MEK at 91.5 % and acetaldehyde at 90.4 %. A recirculation rate (QR) of 50 % improved the system efficiency, particularly for acetaldehyde (49.47 %–63.86 %) and toluene (79.05 %–95.89 %). It also increased the complete energy yield and the selectivity for carbon monoxide (CO) and carbon dioxide (CO2). By-product ozone concentration decreased significantly with increasing recirculation rate at the same input energy level.

- **Keywords:** Volatile organic compounds; Surface DBD; Gas recirculation; Non-thermal plasma

Weiwei Guo, Bo Wu, Qianru Chen, Gul Muhammad, Tianqi Li, Jie Zhang, Junfeng Wan, Yan Wang. *A novel removal strategy of gaseous o-chlorotoluene with UV-activated persulfate sodium in a lab-scale bubble reactor*. Pages 37-46.

Volatile organic compounds (VOCs) from the industries have gotten certain attention; specially the o-chlorotoluene has some serious effects on the ecosystem, as well as on the human nervous and respiratory systems. Therefore, the sodium persulfate (PS) solution irradiated by ultraviolet (UV) was proposed to remove the toxic o-chlorotoluene in this study. The present study focused on the removal efficiency of gaseous o-chlorotoluene and degradation mechanisms. The preliminary results revealed that the removal efficiency was mainly favored by PS concentration, initial pH, UV wavelength and power, inlet o-chlorotoluene concentration, and total gas flow rate. The maximal removal efficiency of gaseous o-chlorotoluene was achieved 93.98 % under optimal experimental conditions. In order to reveal the potential degradation mechanisms, EPR analysis confirmed that both OH and SO4•− were detected during the reaction, and SO4•− acted as the dominant radical for gaseous o-chlorotoluene removal. This study demonstrated that the UV/PS process is an efficient method for removing o-chlorotoluene.

- **Keywords:** Ortho-chlorotoluene removal; Ultraviolet; Sodium persulfate; Scrubber; Mechanism study

Jianbo Yu, Xuefeng Yan. *A new deep model based on the stacked autoencoder with intensified iterative learning style for industrial fault detection*. Pages 47-59.

Deep learning-based process monitoring methods utilize the features extracted from deep neural networks to perform fault detection and diagnosis. Traditional deep learning models are constructed in a fully connected manner and stacked by a sequential connection style. However, the feature information of the observed data would be discarded as the information is compressed and propagated layer-by-layer in hidden layers. Motivated by this, an intensified iterative learning (IIL) model which is developed from the stacked autoencoder is proposed in this study. In the process of feature extraction of IIL model, the traditional constraints of the hidden layer connection in deep neural networks are disregarded and the feature information of the current hidden layer comes from the information of all previous hidden layers to avoid the loss of information. In the process of real-time process monitoring, the features which are advantageous to accomplish fault detection would be intensified to obtain the most favorable features for monitoring. Finally, Euclidean distance and reconstruction error are employed to indicate and visualize the process status. The monitoring performance of the proposed IIL model is evaluated on three process tasks, and the results show it outperforms other deep learning methods on fault detection.

- **Keywords:** Process monitoring; Stacked autoencoder; Intensified iterative learning model; Information loss; Feature information intensify

Anna Crivellari, Sarah Bonvicini, Alessandro Tugnoli, Valerio Cozzani. *Key performance indicators for environmental contamination caused by offshore oil spills*. Pages 60-74.

Oil spills during offshore operations are likely to cause severe contamination of the sea. The identification of the environmental effects of accidental releases from offshore oil and gas facilities plays a crucial role in the prevention and mitigation of marine pollution. Key

Performance Indicators (KPIs) are largely recognized as an effective tool to address and communicate multifaceted issues related to accidental events in the framework of risk management. In the context of Oil Spill Risk Assessment (OSRA) studies, this study proposes a set of KPIs addressing the potential environmental contamination caused by on-surface oil spills from offshore oil and gas installations. A layered approach was defined, based on three different levels of KPIs having an increasing complexity and providing an increasing amount of information. The environmental KPIs defined allow a preliminary quantitative assessment of the environmental contamination due to the oil spill scenarios defined in the ENVironmental hazards IDentification (ENVID) studies carried out for oil and gas installations, providing a preliminary ranking of the expected environmental effects of the spills and supporting their prioritization in order to select those which should undergo a more accurate Environmental Risk Assessment study (ERA).

- **Keywords:** Offshore oil spills; Environmental contamination; KPI; Oil installations; Gas installations; Risk assessment

Jing Yuan, Maria Elektorowicz. *Factors influencing non-aqueous extraction process of bitumen to mitigate the environmental impacts*. Pages 75-83.

Environmental pollutants' transport through tailing extraction process is a big challenge. Hazardous materials in tailings ponds increase with high negative environmental impacts. In this paper, a new type of bench no-water-extracted bitumen process was developed. Factors such as three oil sand ores, namely high, medium, and low-grade in the Athabasca deposits have been exposed to five different light hydrocarbon solvents. The bitumen recovery efficiency of the novel system was investigated with respect to solvent-to-bitumen ratios (S/Bs) as well as solvent and ore properties. The results showed that this novel bench-scale non-aqueous extraction process could significantly reduce water consumption and improve solvent recycling and reduce the release of major hazardous chemicals to oil sands tailings water. The new solvent recovery and bitumen quality for all treated ores were as good as the outcomes from hot water leaching and naphtha froth treatment. When low boiling point solvents (especially cyclopentane) are used to treat high grade ores, the efficiency of bitumen recovery was able to reach over 99 % wt % (by weight %). At the same time, the solvent loss rate could be controlled below 4 barrels (bbl) of solvent per 1000 bbl of extracted bitumen (0.4 %). This indicates the evident effectiveness of non-aqueous extraction of bitumen to mitigate the environmental impacts.

- **Keywords:** Solvent extraction; Oil sands; Non-aqueous system; Environmental impacts; Water management

Ali Farzaneh, Naser Saghatoleslami, Yahya Feyzi. *Transient H2S content rise in the effluent of a natural gas treating unit: Role of COS hydrolysis and heat stable amine salts*. Pages 84-93.

In response to expanding requests towards natural gas usage as a key energy source and vital feedstock, revamping current gas refineries to provide additional capacity and meet the sustainability limitations is considered a crucial essence. In this work, the behavior of a gas refinery after switching its amine solution from diethanolamine to methyldiethanolamine was evaluated. The plant's main goals by this change, i.e., increase sweetening capacity and lowering energy consumption intensity was fulfilled. However, after some overhaul services, the hydrogen sulfide content of final treated gas raised from permissible limit, i.e., 3 ppm at least for three initial months of operation, and then progressively reduced to around 2 ppm. Systematic investigation of plant data shows that carbonyl sulfide hydrolysis in the dehumidification section as downstream of the sweetening section would increase the hydrogen sulfide content of the treated

stream. Meanwhile, the gradual formation of heat stable amine salts in amine solution promotes its absorption capacity, which can counterpoise the effect of further hydrogen sulfide generation due to carbonyl sulfide hydrolysis in the subsequent section. Monitoring heat stable amine salts concentration in amine solution suggests that there should be a minimum level of 0.25 wt.% of these compounds to achieve suitable hydrogen sulfide content in final treated gas.

- **Keywords:** Methyldiethanolamine; Revamping; Heat stable salt; Hydrogen sulfide; Carbonyl sulfide; Hydrolysis

Danilo Bertagna Silva, Gianluigi Buttiglieri, Tomislav Babić, Lidija Ćurković, Sandra Babić. *Impact of UV-LED photoreactor design on the degradation of contaminants of emerging concern*. Pages 94-106.

Recent developments in UV-LED technology open up new possibilities for water treatment. TiO2 photocatalysis can benefit from optimized photoreactor design to increase hydroxyl radical production and reduce its electrical energy per order (EEO) demands, which still ranks high among advanced oxidation processes. However, literature on UV-LED photoreactor design is largely lacking. In this work, a detailed investigation of photoreactor design is proposed. The simulation of a lab scale cylindrical reactor with 8 different UV-LED arrays was run with the professional version of an optic software. The increase of radiant flux and irradiance on the reactor's middle cross section and side walls, respectively, was related to an increasing number of LEDs and to a shorter distance from the reactor but not necessarily to an increase in homogeneity of light distribution. A full factorial experimental design was applied to evaluate the degradation of a representative contaminant of emerging concern (ciprofloxacin) considering 4 independent variables and their interactive effects on kinetic rates and EEO values. The significance of these effects was evaluated with ANOVA and a prediction model was established. The results show that the presence of a TiO2 nanofilm was the most significant tested effect. The number of LEDs, their distance from the reactor's wall and the adoption of controlled periodic illumination also greatly influenced kinetic rates but were less relevant for reducing EEO values because the energetic trade-off was not sufficient to turn the kinetic gain into lower electricity demands.

- **Keywords:** Photoreactor design; Light-emitting diodes; Ciprofloxacin; Design of experiments; Photocatalysis; TiO2

Wancang Liu, Haibo Xiang, Joseph Shiloach, Tao Zhang, Wenni He, Xu Pang, Jing Su, Hongyu Liu, Baiping Ma, Liyan Yu. *Efficient biocatalysis of trillin through recombinant enzyme hydrolysis for clean diosgenin production*. Pages 107-116.

Diosgenin has been widely used as a precursor in the pharmaceutical industry. The conventional diosgenin production method, direct acid hydrolysis, can cause severe environmental pollution and has low production efficiency. In this study, the β-glucosidase FBG1 was successfully over-expressed in Pichia pastoris. The engineered yeast was grown in 5- and 50-L bioreactors to a high-cell-density, and the resulting recombinant FBG1 without purification was directly used for trillin biocatalysis. A novel enzymatic biocatalysis method was established through efficient biocatalysis of trillin by recombinant FBG1 and a practical diosgenin purification process. Diosgenin production reached ~1.7 mg/mL under optimized biocatalysis conditions with a corresponding ~94 % trillin conversion. The production process was further scaled up from 2 mL to 20, 200, and 2000 mL working volumes, producing equivalent efficiency. This recombinant enzyme biocatalysis process resulted in ~680 mg diosgenin when 1 g trillin was processed, together with ~90 % environmental impact elimination and ~36 % cost reduction. Enzymatic biocatalysis can convert trillin into a high-value-added

pharmaceutical precursor of diosgenin with high eco-efficiency, cost-effectiveness, and sustainability is presented here for the first time and is a promising method for future applications in industrial processes.

- **Keywords:** Trillin; Recombinant β-glucosidase; Enzymatic biocatalysis; Diosgenin; Pichia pastoris; High-value-added product

Rong Sun, Wanqi Gong, Yaxian Chen, Junming Hong, Yan Wang. *Influence of polarity exchange frequency on electrokinetic remediation of Cr-contaminated soil using DC and solar energy*. Pages 117-129.

Electrokinetic remediation (EKR) is a remediation method that can effectively remove heavy metals from soil. Traditional EKR uses an external power source to consume electrical energy, in the present study, through the experiment of different electrode exchange frequency to remediate Cr contaminated soil, the effect of polarity exchange electric remediation and the influencing factors of Cr(VI) to Cr(III) conversion are discussed. Five experiments were conducted using DC power supply with conventional EKR (T1), DC power supply with polarity exchange EKR (T2, T3) and solar energy with EKR (T4, T5). The results showed that the T1 experiment had the maximum removal rate of total Cr (42.03 %) and Cr(VI) (85.50 %) but had an adverse effect on soil pH. T2, which exchanged polarity every 24 h, and T3, which exchanged polarity after 84 h, had smaller adverse effects on soil pH, but the removal efficiency was reduced due to repeated migration. The reduction of Cr(VI) to Cr(III) occurred during the EKR processes, the content of Cr(III) increased greatly. Furthermore, few differences were observed between DC power and solar power on the EKR experiments. Therefore, the combination of electrokinetics and solar energy is a feasible method for Cr-contaminated soil.

- **Keywords:** Electrokinetic remediation; Cr-contaminated soil; Polarity exchange; Solar energy

Yonglong Yang, Qiufeng Su, Chenghang Zheng, Yifan Wang, Lingyu Shao, Yue Zhu, Xiang Gao. *Design and development of an ammonia slip detection device and system for flue gas denitration equipment*. Pages 130-138.

An NH3 slip detection device and system were designed and developed. The system includes sampling, absorption, detection, dosing, cleaning, and control components. The problems accompanying low NH3 slip, easy adsorption and instability, can be effectively overcome by the developed device. Furthermore, an online accurate measurement of NH3 slip was realized. Meanwhile, the online calibration function of the device addresses the drawbacks of existing online NH3 slip monitoring devices. The reliability and stability of the detection data were improved, whereas the sampling time, flow rate, gas concentration, and pH, which affect the NH3 measurement results, were experimentally investigated. The main sampling parameters were optimized by orthogonal experiments, and the measurement error of the detection device was obtained according to experimental results. A correction model for measured values was then established, which further improved the accuracy of the measured data. The device has the advantages of high efficiency, stability, high accuracy, online calibration ability, and high integration compared with existing NH3 slip detection devices for denitration systems. The developed device can be utilized for online detection of NH3 slip in the denitration equipment of coal-fired power plants.

- **Keywords:** Coal-fired power plant; NH3 slip; Detecting device; Checkout; Design

Miaomiao Qu, Zhuowei Cheng, Zhirong Sun, Dongzhi Chen, Jianming Yu, Jianmeng Chen. *Non-thermal plasma coupled with catalysis for VOCs abatement: A review*. Pages 139-158.

Volatile organic compounds (VOCs) emitted from various industrial processes are extremely harmful pollutants. They are involved in the formation of ozone, photochemical smog, and fine particles (PM2.5) in the atmosphere, which pose considerable threat to human healthy and ecosystem safety. The hybrid plasma-catalytic technology that uses non-thermal plasma (NTP) and catalysts is an efficient method for VOC abatement. This review provides a comprehensive insight into the removal of VOCs with this technology. First, the synergistic effects and mechanisms of NTP and catalysts are discussed. Then, the properties of the catalysts, including types, positions, and other parameters, are explored. Specific examples of VOCs abated using the NTP-catalyst technology are reviewed, along with the main types and the causes of by-products. Several methods, such as the optimization of process parameters and the utilization of end control, are considered efficient for the regulation of product formations. Finally, future perspectives on the applications of this hybrid technology are briefly discussed.

- **Keywords:** Non thermal plasma-catalyst; Synergistic mechanism; By-product; VOC abatement

Jian Chen, Yanli Zhao, Yubo Bi, Changhai Li, Depeng Kong, Shouxiang Lu. *Effect of initial pressure on the burning behavior of ethanol pool fire in the closed pressure vessel*. Pages 159-166.

Fire Hazards associated with pressure vessel seriously threaten the process safety in chemical industries. There are limited literatures about fire characteristics in closed pressure vessels, which are important for fire risk management and safety design. In this study, the effect of initial pressure on the burning behavior of ethanol pool fire in a pressure vessel was investigated. A series of ethanol pool fires with diameters from 4 cm to 10 cm was carried out in a pressure vessel with interior dimensions of 0.6 m (height) ×0.4 m (diameter), and the initial pressures range from 60 kPa to 300 kPa. Results show that the flame structure changes from laminar to turbulent and the flame color changes from yellow to blue as the initial pressure or the burning time increases, which can provide information on the flow and chemical details. Furthermore, considering the effect of initial pressure on the mean burning flux, an empirical formula for predicting the self-extinction time of pool fire in the closed pressure vessel was developed, which showing a good agreement with the experimental data in our study and previous tests. Finally, it was observed that the changes of pressure with time are similar to the change of mass burning rate and could be divided into three representative stages. The relationship for predicting the over pressure peak was introduced and verified by the experimental data.

- **Keywords:** Pool fire; Initial pressure; Closed vessel; Burning behavior

Tianshu Xu, Zhoumo Zeng, Xinjing Huang, Jian Li, Hao Feng. *Pipeline leak detection based on variational mode decomposition and support vector machine using an interior spherical detector*. Pages 167-177.

A spherical detector (SD) is capable of closely approaching a leak point and collecting leak sounds from the inside of a long pipeline, thereby enabling an extremely high leak detection sensitivity. However, acoustic noises arise from collision and friction while the SD is rolling forward, hindering the identification of leak acoustic signals. To address this challenge, this work presents a pipeline leak identification method for an SD based on combining variational mode decomposition (VMD) and a support vector machine (SVM). A leak generation system is set up where the pipe is water-filled, pressurized, and tiltable, and the SD can stand still or roll to collect a sufficient variety of leak sound

samples. By decomposing the noisy signals into different modes and selecting the modes with high correlations to reconstruct the signals, the VMD can significantly decrease the collision noise. Additionally, the Mel frequency cepstral coefficients (MFCCs) are extracted and used to constitute a characteristic vector for SVM-based leak recognition. The trained neural network effectively identifies the occurrence of a leak; the recognition accuracy can reach up to 93 %, with a satisfactory specificity of 89.6 %.

- **Keywords:** Pipeline; Leak detection; Spherical detector; Signal de-noising

Lakshmi N. J., Parag R. Gogate, Aniruddha B. Pandit. Treatment of acid violet 7 dye containing effluent using the hybrid approach based on hydrodynamic cavitation. Pages 178-191.

The present work investigates the degradation of the azo dye, Acid violet-7 using hydrodynamic cavitation (HC) in combination with advanced oxidation processes (AOPs). The recalcitrant nature of the dye makes the conventional methods of degradation less effective and hence it is important to explore advanced methods. The development of treatment scheme for AV-7 using HC involved the optimization of initial dye concentration (10–200 ppm) and operating pH (3–10) to maximize decolorization using the approach of HC alone. At the optimum initial dye concentration of 20 ppm, operating pH of 3 and selected inlet pressure of 4 bar, the maximum decolorization was 39.1 % and mineralization was 25.2 % obtained using individual HC process without the addition of any chemical oxidants. The combined process of HC coupled with oxidants evaluated in the work were HC+H2O2, HC + KPS and HC + Fenton which resulted in the extent of decolorization as 70.49, 77.72 and 94.02 % respectively and the extent of mineralization as 38, 48.8 and 70.4 % respectively. The dye decolorization followed first order kinetics in all the approaches and obtained rate constants were used to evaluate the effectiveness of combinations in terms of the synergistic index. Additionally, comparison of efficacy of each treatment scheme was established with the aid of cavitational yield and the treatment costs. Overall, the combination of HC and Fenton oxidation was demonstrated to be the best approach for the degradation of AC-7 dye compared to the other combined oxidation processes.

- **Keywords:** Acid violet-7; Hydrodynamic cavitation; Advanced oxidation process; Synergistic index; Cavitational yield

Namil Um, Tae-Wan Jeon. Pretreatment method for the utilization of the coal ash landfilled in ash ponds. Pages 192-204.

The coal ash (CA) generated from coal-fired power plants (CPPs) is collected in ash ponds (APs), most of which are actually full, so there are concerns regarding the potential contamination of the environment around them. Thus, in the present study, a method for improving the utilization of coal pond ash (CPA) was proposed. Here the CA landfilled in an AP was regarded as CPA. Furthermore, the CPA characteristics (particle size and weight distributions, chemical composition, unburned carbon (UC) content, particle image, and mineralogical analysis) were investigated. Next, experiments were conducted on the main separation processes: screening with five standard sieves having 0.15-, 0.3-, 0.6-, 1.18-, and 2.36-mm diameter grids; float–sink experiments with four different specific gravities (SGs) of under 1.8 SG, 1.8–2.2 SG, and 2.2–2.5 SG and over 2.5 SG; flotation with a column-type glass reactor under the conditions of pH 2, 7, and 12; grinding with a batch-type ball mill for 5, 10, 20, and 40 min; wet magnetic separation with four magnetic forces (0.1, 0.5, 1, and 2 T). Based on these results, a pretreatment method was proposed and the final materials could be categorized into UC, amorphous compounds (ACs) with Al species (Al2O3·xH2O) and glassy phases, inorganic materials with Si and Al, and ferrous material groups. Besides, six additional pretreatment methods were suggested through various combinations of each separation process. As a case of

South Korea, the applicability of this method to the entire CPA in South Korea was also confirmed.

- **Keywords:** Coal pond ash; Pretreatment method design; Flotation; Float-sink; Magnetic separation

Kushal Adhikari, Clifford B. Fedler, Alireza Asadi. *2-D modeling to understand the design configuration and flow dynamics of Pond-In-Pond (PIP) wastewater treatment system for reuse*. Pages 205-214.

Water reuse for irrigation is increasingly recognized as an essential and economical strategy in areas with water scarcity. A simple, low cost, low-maintenance, and highly efficient Pond-In-Pond (PIP) treatment system can be used for wastewater reuse. PIP is a treatment technology in which two types of ponds -- anaerobic and aerobic -- are combined into a single pond and consists of a deeper inner section entirely submerged within the outer pond. Previous studies on PIPs and PIP-like systems have reinforced the potential for reuse through promising performance results with BOD removal over 80 % and a reduction in land area requirements by approximately 40 %. Yet, no prior efforts have been made to understand the performance mechanism of such systems. This study makes use of two, 2-D modeling tools in developing a fundamental understanding of PIP flow dynamics and the expected performance. The modeling results showed that the PIP configuration offers improved flow-diversion along with reduced flow velocity. Additionally, the PIP retained approximately 17 % more ($p < 0.05$) particles than the traditional pond with most of the particles concentrated within the inner pond. Lower velocity and the higher solids retention in the PIP thus allowed for better treatment performance compared to traditional ponds. The findings from this study can be used as preliminary data for future in-depth investigations of the PIP system leading toward effective and optimal designs. This will help address the major societal concern of water scarcity with low-cost and effective wastewater treatment.

- **Keywords:** Wastewater reuse; Irrigation; Sustainability; Pond-In-Pond; Pond configuration; 2-D modeling

Toktam Ghadam Soltani, Mansour Mashreghi, Mohammad Reza Housaindokht, Mohamad Hosein Mahmudy Gharaie. *Modelling and characterization of an engineered microbial biosensor for high-throughput screening of arsenic in rural water*. Pages 215-224.

Current arsenic analysis methods in groundwater samples rely on expensive apparatus, complicated procedures, and dangerous chemical reagents. Also, delays in detecting arsenic harm to public health, the environment, agriculture and food sectors. Therefore, in this study, a bioluminescent biosensor has been optimized and used to detect and measure arsenic concentration in groundwater. Optimum conditions for the appropriate performance of E. coli DH5α (pJAMA-arsR) were determined and the luminescent calibration curve was drawn. The optimization results showed that maximum luminescent light output could occur at the end of the logarithmic phase or the beginning of the stationary phase, the temperature of 37 °C, and pH between 5.5 and 7 upon adding 10 µl n-decanal (18 mM). Increasing the duration of bacterial induction by arsenic leads to elevation of biosensor luminescent light yield. Functional stability of the biosensor with 20 % glycerol (V/V) at −20 °C was verified for at least six months. Luminescence reaction of the bacterial biosensor cells to arsenic concentration in the range of 0–90 ppb was promising ($R2 = 0.948$ by linear regression), but higher arsenic concentration had poisonous effect on biosensor cells. The modified Gompertz model derived here could successfully predict the bacterial biosensor growth under the optimum condition compared with experimental data. In this study critical challenges, such as technical and appropriate performance, are defined to interpret the bacterial biosensor's true

perspective to promote its broad adoption and usage. The work is concluded with closing remarks and potential perspectives to emphasize the importance of the bacterial biosensor, which could detect arsenic from a wide scope in real-time, quickly, and environmentally friendly signaling tool with high sensitivity and selectivity.

- **Keywords:** Biosensor; Arsenic; Gompertz model; Growth kinetics; E. coli DH5α (pJAMA8-arsR)

Xueqiang Shi, Yutao Zhang, Xiaokun Chen, Yuanbo Zhang, Qian Ma. *Characteristics of coal dust ignited by a hot particle*. Pages 225-238.

Ignition of coal dust caused by hot particles (ICDHP) will lead to serious combustion or explosion. In this work, the coupling details of multi–physical fields of the ICDHP were established. Two different chemical reactions of flaming combustion of volatiles and smoldering of coal dust were established to understand the mechanism and process of the ICDHP. The evolution of temperature, volatiles molar concentration and heat release characteristics under different particle temperatures and contact conditions between the hot particle and coal dust were investigated. Results show that there are two ways of the ICDHP, which are volatiles ignition and coal smoldering ignition. The ignition delay time (IDT) increases exponentially with the decrease of the hot particle temperature. The temperature of the hot particle is 1100 K, and thermal runaway occurs in the way of coal smoldering ignition. When the temperature of the hot particle is higher than 1100 K, thermal runaway occurs in the way of volatiles ignition. In addition, it is found that the IDT decreases exponentially with the increase of the buried depth (lp) of the hot particle in coal dust for the hot particle temperature of 1186 K. The IDT shows a trend of decreasing – increasing – decreasing with the increase of lp for the hot particle temperatures of 1271 K and 1369 K. If the hot particle is completely embedded in the coal dust, the smoldering combustion of the coal dust is found. In addition, the volatiles first react on the side of the hot particle, and the thermal runaway occurs at the position where the concentration and temperature of volatiles are high enough.

- **Keywords:** Ignition; Coal dust; Volatiles; Numerical simulation; Hot particle

Anup Kumar Singh, Vediappan Sudhakar. *Highly efficient method of utilizing waste silica hazards*. Pages 239-248.

Silica gels are the significant commodity solid waste produced by organic laboratories and pharmaceutic industries. Although use of silica gels is continuously growing, the proper methods of re-utilizing silica waste are yet limited. Hence, it demands a non-traditional approach to transform these silica waste into some other useful products apart from using them as a well-known road construction materials. Hereby, we report the fabrication and applications of monolithic polymer-silica composites by ice-templating technique from laboratory waste silica-gels, using green approach. To the best of our knowledge, the fabrication of organic-inorganic hybrid sponges from the particles of hundreds of microns is not reported to date. Scaffolds S60, S120, S180, and S300, were prepared from laboratory discarded silica gels. The morphological, physicochemical, flame-retardant, and liquid absorbent properties of these self-standing scaffolds were analyzed. Results showed that the incorporation of silica particles in the scaffolds turned them into a flame-retardant sponge. These properties make the sponges ideal for making non-flammable cushions, applicable in automobiles, aircrafts, chemical laboratories, hospitals, and other areas of applications. Due to the large porous structures, these scaffolds possess excellent absorption properties and may absorb almost every kind of liquid ranging from oils to acids. Therefore, these scaffolds are also a remarkable absorber for oils and hazardous liquids spillage, such as acids, and can be used as foam for chemical packing applications.

- **Keywords:** Laboratory silica waste; Scaffolds; Ice-templating; Flame-retardant; Acid absorber

Jiawei Cui, Lei Ni, Juncheng Jiang, Shuliang Ye, Saili Shen, Mengya Zou. *Numerical simulation of the thermal decomposition of tert-butyl peroxyacetate in adiabatic tests*. Pages 249-256.

Adiabatic calorimeters (ARCs) are critical in thermal analysis and thermal hazard assessment. As testing equipment continually improves, analyzing changes in physical fields in sample pools during thermal decomposition reactions is increasingly essential. Therefore, this study analyzed the thermal decomposition of tert-butyl peroxyacetate (TBPA). On the basis of the computational fluid dynamics (CFD) numerical simulation method and the kinetic model of TBPA thermal decomposition, a full-scale model of an adiabatic reactor for the thermal decomposition of TBPA was constructed. The temperature rise curve obtained after monitoring the temperature of the system during thermal decomposition was compared with that obtained during the experiment; thus, the rationality of the CFD model was verified. Accordingly, the temperature field, temperature rate, and velocity field in the reactor were analyzed. The temperature distribution of the system was relatively uniform during thermal decomposition under completely adiabatic conditions, resulting in an effectively nonexistent temperature gradient. At the same time, the self-heat rate (dT/dt) of the system in the process of thermal decomposition was analyzed. It was found that self-heat rate (dT/dt) of the system in the full sensing state was much larger than that in the experimental process, maximum self-heat rate ((dT/dt)max) reaching 15℃/min, while in the experimental process was only 1.074℃/min.

- **Keywords:** Adiabatic calorimeter; Computational fluid dynamics; Tert-butyl peroxyacetate; Thermal decomposition reaction

Boqian Li, Shu Li, Ludong Yi, Haosheng Sun, Jun Qin, Jun Wang, Dawei Fang. *Degradation of organophosphorus pesticide diazinon by hydrodynamic cavitation: Parameters optimization and mechanism investigation*. Pages 257-267.

Diazinon (DZN), a broad-spectrum and highly effective organophosphorus pesticide, is widely being used in agricultural production and household environments. However, massive DZN effluent can be generated during the DZN production process, which will cause devastating effects on the ecosystem and damage human health due to the improper dispose of pesticide effluent before discharging. In this work, hydrodynamic cavitation (HC), a new advanced oxidation technology, was used to degrade DZN in wastewater for the first time. The influences of DZN initial concentration (5.0–15 mg/L), solution pH (4.0–10), temperature (30–50 °C) and some orifice plate geometric parameters (orifice numbers and orifice half angles) on the degradation effect of DZN were investigated. It can be observed that the DZN in solution can be effectively degraded in orifice plate HC system based on three orifices with 45° convergent half angle and the degradation ratio can reach 50.52 % under the operation conditions of 150 min treatment time, 30 °C temperature and pH = 4.0 acidity. Subsequently, the studies of intensifying DZN degradation were also carried out through adding different inorganic oxidants such as potassium peroxodisulfate (K2S2O8), potassium periodate (KIO4) and sodium perchlorate (NaClO4). The maximum DZN HC degradation extent (81.92 %) can be achieved in the presence of K2S2O8 under the optimized conditions. The generated intermediate products in DZN HC degradation process are some low-toxic and low-active substances. And that, these intermediate products can be further mineralized to H2O, CO2 and inorganic ions. On the basis of cavitational yield, the energy consumption analysis has been performed. Overall, this work demonstrates that the HC

combined with oxidant K2S2O8 may be a promising strategy for the large-scale treatment of organophosphorus pesticide wastewater.

- **Keywords:** Hydrodynamic cavitation (HC); Orifice plate; Inorganic oxidants; Organophosphorus pesticide; Degradation; Mineralization

Jing-Wen Luo, Qiu-Hong Wang, Yi-Hung Chung, Vikranth Volli, Chi-Min Shu, Yu-Chi Cheng. *Hazard evaluation, explosion risk, and thermal behaviour of magnesium- aluminium alloys during the polishing process by using a 20-L apparatus, MIEA, and TGA*. Pages 268-277.

Magnesium-aluminium alloy powders, although widely used in the polishing process on variable scales, also have a potential to be explosive. Having a thorough understanding of the thermal aspects of magnesium-aluminium alloy powder ensures process safety and is essential for developing an adequate emergency system. This study analysed the influence of the particle size, ranging between 105 and 420 μm on the thermal characteristics of magnesium-aluminium. The results revealed that at a dust concentration of 1750 g/m3, 105, 210, and 420 μm magnesium-aluminium alloy powders exhibited a maximum explosion pressure of 0.97, 0.86, and 0.78 MPa, respectively. The limiting oxygen concentration values of 105, 210, and 420 μm samples were 4, 13, and 15 vol.%, respectively. The apparent activation energies Ea of 105, 210, and 420 μm samples were 286.5–70.6, 165.2–39.9, and 224.8–168.8 kJ/mol, respectively. Furthermore, the flammability parameters exhibited greater reactivity for smaller particle sizes, i.e., the minimum ignition temperature sharply decreased from 700 to 550 °C. Thus, this study provides valuable insights into the combustion characteristics and the severity of the dust explosion hazards of magnesium-aluminium alloy powders in order to ensure better safety standards in the metal processing industry.

- **Keywords:** Limiting oxygen concentration; Apparent activation energies; Flammability parameters; Minimum ignition temperature; Dust explosion hazards

Maureen Heraty Wood, Mark Hailwood, Konstantinos Koutelos. *Reducing the risk of oxygen-related fires and explosions in hospitals treating Covid-19 patients*. Pages 278-288.

On 24 April a disastrous fire in an Iraqi hospital took the lives of 82 people. Since the outbreak of the pandemic in March 2020, incidents of oxygen-related hospital fires in various countries around the world have caused over 200 deaths, the majority of whom were patients extremely ill with the novel Coronavirus. Fires involving medical oxygen are not a new phenomenon but are more common in the operating theatre where oxygen is routinely administered. In these settings, strict safety protocols are normally enforced and surgical staff are well trained in dealing with oxygen hazards. It appears that some hospitals may not have been fully prepared for the elevated risk of oxygen-related fire in intensive care units due to the high demand for oxygen therapy in severely ill Covid-19 patients. Indeed, gas producers and public health authorities were also slow to recognize and alert hospitals to the potential dangers. Oxygen is essential to life and generally makes up about 21 % of the gases in the air we breathe. Pure oxygen reacts with common materials such as oil and grease to cause fires, and even explosions, when released at high pressures. A leaking valve or hose, and openings at interfaces of masks and tubes, when in a confined space or where air circulation is low, can quickly increase the oxygen concentration to a dangerous level. Even a small increase in the oxygen level in the air to 24 % can create a fire hazard. In an oxygen-enriched environment, materials become easier to ignite and fires will burn hotter and more fiercely than in normal air. There is also a potentially heightened risk of using ethanol-based and organic solvents as cleaning agents in an oxygen rich atmospheres. This paper will provide an overview of oxygen accident scenarios that may be relevant for hospital intensive care

units, with particular reference to recent events and similar accidents that have occurred in the past. The paper will recommend that hospitals recognize their chemical risks as part of their risk governance responsibility and assign chemical risk management a prominent role in their overall management. Investigation of dangerous events to extract causes and lessons learned should be utilized to highlight opportunities for prevention as well as emergency response. The industrial gas industry also needs to actively support hospitals in adoption of more rigorous risk management approaches, building on lessons learned in chemical process safety for managing flammable and explosive atmospheres.

- **Keywords:** Covid-19; Oxygen enriched atmosphere; Hospital fire; Intensive care; Fire safety + prevention; Oxygen hazard

Didier Ramírez-Morales, Mario Masís-Mora, José R. Montiel-Mora, Juan Carlos Cambronero-Heinrichs, Greivin Pérez-Rojas, Rebeca Tormo-Budowski, Michael Méndez-Rivera, Susana Briceño-Guevara, Juan Antonio Gutiérrez-Quirós, Víctor Arias-Mora, Laura Brenes-Alfaro, Wilson Beita-Sandí, Carlos E. Rodríguez-Rodríguez. *Multi-residue analysis of pharmaceuticals in water samples by liquid chromatography- mass spectrometry: Quality assessment and application to the risk assessment of urban-influenced surface waters in a metropolitan area of Central America*. Pages 289-300.

The occurrence of pharmaceuticals in surface water has been barely studied in Latin America. This work aimed to i) develop a multi-residue liquid chromatography- triple quadrupole mass spectrometry (LC–MS/MS) method for the determination of pharmaceutical active compounds (PhACs); ii) monitor 70 PhACs in three urban-influenced rivers in San José, Costa Rica; and iii) perform the risk assessment of detected compounds and ecotoxicological evaluation on water samples. Caffeine, 1,7-dimethylxanthine, naproxen, gemfibrozil and ibuprofen were the most frequent among 23 detected compounds. Concentrations ranged from 0.013 μg/L to 53.8 μg/L (62 % detections between 0.1 μg/L–1 μg/L), and the highest values corresponded to caffeine, 1,7-dimethylxanthine, ofloxacin, gemfibrozil and cephalexin. The environmental risk estimated using the hazard quotient (HQ) approach, revealed four and eleven compounds with medium and high risk, respectively. The highest risk (HQ >10) was determined for diphenhydramine, risperidone, fluoxetine, trimethoprim, ofloxacin and azithromycin; nonetheless, high risk (HQ >1) was also estimated for caffeine, diclofenac, clarithromycin, gemfibrozil and ibuprofen. Total HQ sample values (ΣHQ), calculated as the sum of individual HQs for each detected compound, revealed the highest hazard in surface water near wastewater treatment plant discharges, followed by the locations of higher urban influence (in the Virilla river). Ecotoxicological evaluation showed no acute toxicity towards Daphnia magna and Vibrio fischeri in surface water samples; on the contrary, toxicity towards Lactuca sativa (germination tests) showed a similar pattern to that determined with the ΣHQ, although the highest toxicity was observed downstream with respect to the urban influence of the metropolitan area. These findings help to visualize the importance of pharmaceutical residues in the overall toxicity of surface water samples, and remark the relevance of monitoring these compounds, as an input for the implementation of future mitigation actions.

- **Keywords:** Analytical validation; Ecotoxicity; Hazard quotient; Anthropogenic pollution; Environmental risk

Tobias Reinhardt, Eduard Rott, Philip A. Schneider, Ralf Minke, Harald Schönberger. *Fixed-bed column studies of phosphonate and phosphate adsorption on granular ferric hydroxide (GFH)*. Pages 301-310.

The use of phosphonates as antiscalants in membrane processes is common. Before they are discharged into the receiving water, they should be removed from the membrane concentrate to protect the aquatic environment. This study conducted fixed-bed column experiments on the adsorption of diethylenetriaminepenta(methylene phosphonic acid) (DTPMP) and ortho-phosphate on granular ferric (hydr)oxide (GFH). The objective was to investigate the adsorption and desorption performance using real membrane concentrate, while testing both the usability of the GFH and that of the regeneration solutions over multiple cycles. Whereas a synthetic solution with DTPMP allowed almost complete regeneration, the adsorption performance with real membrane concentrate at the original pH ≅ 8 decreased significantly. This could be attributed to the precipitation of calcium compounds which disturbed the adsorption/desorption process. With the introduction of a novel acidic regeneration step to remove the precipitates, an adsorption performance of 95% over 20 cycles was achieved. The hydrochloric acid (HCl) can be reused when its pH is kept constant by a pH control. The sodium hydroxide solution (NaOH) for alkaline regeneration can be reused several times. However, the desorption performance decreased significantly when its electrical conductivity dropped below 90 mS/cm. Replacing the NaOH regularly can significantly improve the desorption performance.

- **Keywords:** Adsorption; Desorption; Fixed-bed column; Ortho-phosphate; Phosphonates; Regeneration

Shengyong Hu, Yang Gao, Fei Hu, Guorui Feng, Changhe Liu, Jihua Li. *A novel method for cleaning coal-dust-laden air and its application*. Pages 311-319.

During the green mining processes of coal energy, large amounts of coal-dust-laden air may be generated. This has caused serious health threats to mine workers. In this paper, a novel method for efficiently cleaning coal-dust-laden air was proposed. The method involved the use of air scrubbers composed of water inlet pipes, radial mixing impellers, water distribution plates, swirl vanes, and dehydrator. The radial mixing impellers were utilized to break up the water which flowed from the water inlet pipes to water distribution plates. As a result, water mist was formed, which then combined with the coal-dust-laden air, effectively sucking it using the negative pressure from the impeller rotation actions. The coal-dust-laden air and solid-liquid mixtures were moved along a certain trajectory by centrifugal force and gravity, and then discharged to the exterior. Experiments and field application processes were carried out in order to test the effectiveness of the proposed method. The experimental results showed that the dust removal efficiency of the method had reached 97.70 %. In addition, the proposed method was applied to a coal preparation plant in China's Shanxi Province. The test results indicated that the average concentrations of total dust and respirable dust were found to have decreased from 71.11 to 2.89 mg/m3 and from 47.675 to 1.958 mg/m3, which met the requirements of environmental standards. Therefore, since the proposed method had not used conventional nozzles and filters, and had no requirements regarding the water quality of the coal mine, it had displayed strong adaptability and stable dust removal efficiency. The results obtained in this study showed that this new method of cleaning coal-dust-laden air was a promising measure by which to significantly improve the working environments of coal mines.

- **Keywords:** Coal dust; Coal-dust-laden air; Air scrubber; Dust removal efficiency

Zunxiang Qiu, Quanlong Liu, Xinchun Li, Jinjia Zhang, Yueqian Zhang. *Construction and analysis of a coal mine accident causation network based on text mining*. Pages 320-328.

It is important to systematically identify the contributing factors in coal mine accidents from a large-scale analysis of accident reports. However, previous scholars have mainly

used human analysis methods to define accident-causing factors, leading to incomplete and biased cause checklists due to personal experience and knowledge. Furthermore, a data-driven method is needed to quantify the importance of each factor and clarify the mechanism of different types of accidents. Considering these, this study creatively combined text mining technology and a complex network to explore the coal mine accident-causing mechanism. Through the text mining of 307 accident reports, 52 main accident-causing factors were identified, and a coal mine accident causation network was constructed based on the strong association rules among factors. Second, eight core factors and their associated sets, as well as seven critical links for different accident types, were clarified through network centrality analysis and accident path analysis. This study shows that regulatory authority is the most influential level of accident causation, gas accidents are the most easily triggered accident type, a lack of effective mechanism for safety supervision→failure to arrange full-time safety inspectors to follow the shift→lack of serious and thorough on-site hidden danger investigations→inadequate anti-surge measures are the key links in gas accident causation. This study contributes new perspectives on identifying contributing factors and their complex interaction mechanisms from accident report data for practical applications in risk analysis and accident prevention.

- **Keywords:** Coal mine safety; Text mining technology; Complex network theory; Accident causation; Risk analysis

Shiyang Zhang, Jing Chen, Wenjiao Sang, Meng Li, Veljko Prodanovic, Kefeng Zhang. *Metagenomic insights into the explanation of biofilter performance distinction induced by dissolved oxygen inkrement*. Pages 329-338.

In this study, a set of novel double-layer-packed sequencing batch biofilm reactors (SBBRs) were constructed to treat secondary effluent with a low carbon-to-nitrogen ratio (C/N = 3.0). All the reactors were operated under identical conditions except dissolved oxygen (DO) in the aerobic section, which was controlled at seven different levels (0.5, 1.0, 1.5, 2.0, 2.5, 3.5 and 4.5 mg/L). It was found that the aerobic section contributed most to performance at an optimal DO of 2.0 mg/L. The change in DO accounted for the varied bacterial communities, which resulted in different performances. Both bacterial community structure and potential functions displayed close associations with performance implying nutrients were mainly removed by simultaneous nitrification-endogenous denitrification and phosphorus removal (SNEDPR) process. Moreover, the proliferation of nonfunctional nitrifiers/denitrifiers led to the inhibition of denitrification resulting in a lower removal of total dissolved nitrogen and phosphorus.

- **Keywords:** Secondary effluent; Sequencing batch biofilm reactor (SBBR); Simultaneous nitrification and denitrification (SND); Dissolved oxygen (DO); Purification performance

Ahmed Shawki Ahmed, Diego Rosso, Domenico Santoro, George Nakhla. *Influence of substrates concentrations on the dynamics of oxygen demand and aeration performance in ideal bioreactors*. Pages 339-353.

The effect of bioreactor configurations on the dynamics of aeration modelling was investigated by incorporating three different correlations from the literature to estimate α-factors into the aeration model. Estimated air flow rates using the three correlations were then validated against experimental data obtained from pilot sequencing batch reactors (SBRs). Two identical SBRs were operated in parallel; one received raw wastewater and the other received primary treated wastewater. The validated aeration model was then used to evaluate aeration dynamics in different bioreactor configurations, both for nitrification only and nitrification/denitrification, with the three different

correlations. The current study is the first to investigate the validity of the aforementioned correlations using various bioreactor configurations and to establish that the bioreactor configuration not only impacts spatial and temporal biological oxygen demands as currently understood but also oxygen transfer efficiency. The first correlation based on the real-time bioreactor soluble chemical oxygen demand (sCOD) was able to predict the temporal measured air flow rate in the pilot SBRs. The second correlation based on the influent COD overestimated the air flow rates as it considered the impact of the influent loading rates on the α-factor and overlooked the improvement in α-factor due to biodegradation. The third correlation based on MLSS concentrations underestimated the air flow rates at the beginning of the aeration cycle as it ignored the impact of influent loading rates on the α-factor and considered only the insignificant change in MLSS during the aeration cycle. In terms of bioreactor configuration, the model-based analysis showed that the first correlation is suitable for designing SBR, plug flow reactor (PFR), step-feed PFR, and completely mixed stirred reactor (CSTR) systems, and the third correlation is suitable for designing CSTRs and membrane bioreactors (MBRs), while the second correlation was not accurate in any of the reactors modelled. When nitrification was targeted, the CSTR reduced aeration energy by 44 %–49 % compared to the PFR, and 41 %–43 % when both nitrification and denitrification were targeted. Compared to the plug-flow reactor, the step-feed PFR reduced aeration energy by 9% when nitrification only was targeted. However, when pre-denitrification was added, both systems showed the same aeration energy consumption. Pre-denitrification reduced organic loadings to aeration tanks and decreased aeration energy by 22 %, 11 %, 15 %, and 14 % in PFR, CSTR, PFR step feed and MBR systems, respectively.

- **Keywords:** Aeration energy; Activated sludge; Aeration modelling; Bioreactor configuration; Oxygen transfer; α-Factor

Ping Li, Qian Zeng, Qiangling Duan, Jinhua Sun. *Visualization of spontaneous ignition and flame behavior in tubes with and without obstacles during the high-pressure hydrogen release*. Pages 354-362.

This paper studies the effects of triangle obstacles inside the tube on the ignition mechanism and subsequent flame development in a semi-confined space when high-pressure hydrogen sudden release. Smooth tube and obstructed tube with optical glasses are constructed where controlled high-pressure hydrogen are released. High-speed direct photography is used to image the flame evolution while pressure transducers are used to obtain pressure-time traces both inside the tube and exhaust chamber. These cases that hydrogen with various burst pressure jets into the smooth and obstructed tubes are tested. It is found that spontaneous ignition occurs in the boundary layer of the tube in the smooth tube, a complete fire spanning the cross-section is reached as the flame propagates within the mixing region. The appearance of obstacles is found to have a significant effect on the ignition mechanism and flame structure. A two-way dissemination reflected shock wave forms and three possible ignition region emerges surrounding the obstacles. The flame propagation restricted between the leading shock wave and hydrogen jet. The flame experiences a split that the front flame in the vicinity of the obstacle gradually dies out and the rear flame continues propagating within the mixing region. The flame evolution and pressure variation in the exhaust chamber show that obstacles inside the tube do not aggravate the disaster in the semi-confined chamber.

- **Keywords:** High-pressure hydrogen; triangle obstacle; spontaneous ignition; flame behavior

Mohamed Marzouk, Nehal Elshaboury, Amr Abdel-Latif, Shimaa Azab. *Deep learning model for forecasting COVID-19 outbreak in Egypt*. Pages 363-375.

The World Health Organization has declared COVID-19 as a global pandemic in early 2020. A comprehensive understanding of the epidemiological characteristics of this virus is crucial to limit its spreading. Therefore, this research applies artificial intelligence-based models to predict the prevalence of the COVID-19 outbreak in Egypt. These models are long short-term memory network (LSTM), convolutional neural network, and multilayer perceptron neural network. They are trained and validated using the dataset records from 14 February 2020 to 15 August 2020. The results of the models are evaluated using the determination coefficient and root mean square error. The LSTM model exhibits the best performance in forecasting the cumulative infections for one week and one month ahead. Finally, the LSTM model with the optimal parameter values is applied to forecast the spread of this epidemic for one month ahead using the data from 14 February 2020 to 30 June 2021. The total size of infections, recoveries, and deaths is estimated to be 285,939, 234,747, and 17,251 cases on 31 July 2021. This study could assist the decision-makers in developing and monitoring policies to confront this disease.

- **Keywords:** COVID-19; Epidemic model; Deep learning; Long short-term memory network; Egypt

Fatima Elazhar, Maryem Elazhar, Soufian El-Ghzizel, Mustapha Tahaikt, Mohamed Zait, Driss Dhiba, Azzedine Elmidaoui, Mohamed Taky. *Nanofiltration-reverse osmosis hybrid process for hardness removal in brackish water with higher recovery rate and minimization of brine discharges*. Pages 376-383.

In this paper, the feasibility of hybrid nanofiltration-reverse osmosis (NF-RO) process to remove hardness in brackish water at higher recovery rate and concentrate minimization is investigated. Two nanofiltration (NF) membranes are tested in the first stage for selecting the appropriate membrane on the basis of lower applied pressure and higher permeate flow. Then the evaluation of the performances of hybrid NF-RO system of each stage is studied in terms of recovery rate and Langelier saturation index (LSI) values to prevent the corrosion potential. The blending strategy is adopted with NF brine and reverse osmosis (RO) permeate in order to bring the RO permeate characteristics in accordance with drinking water standards and to minimize the volume of NF brine. Also, energy consumption performance of conventional nanofiltration (NF-NF) and NF-RO hybrid system in hardness removal is compared. The results show that the NF-RO hybrid system combined to blending strategy provides the simplest process but most energy efficient process compared to a single conventional NF-NF. Moreover, including NF upstream of RO is responsible of the increasing of the overall water recovery rate (95 %) and of the permeate quality with lower total dissolved solids (TDS). However, less water with lower salinity treated by RO increases significantly the recovery rate in RO stage up to 80 %. The portion rate of NF brine blending with RO permeate is equal to 32.45 %, corresponding to 240L/h, which meet the water quality regulations for drinking water. Hybrid NF-RO system has a lower energy cost per m3 than NF-NF, it is around of 0.055 $/m3. At the same time, this procedure minimizes the fraction of brine disposal dumping to sewage, making it environmentally friendly.

- **Keywords:** Hardness; Hybrid system; Desalination; Langelier saturation index (LSI); Brine disposal

Moeen Gholami, Behrooz Abbasi Souraki, Alireza Pendashteh. *Electro-activated persulfate oxidation (EC/PS) for the treatment of real oilfield produced water: Optimization, developed numerical kinetic model, and comparison with thermal/EC/PS and EC systems*. Pages 384-402.

In this study, the performance and efficiency of electrocoagulation (EC), electro-activation of persulfate (EC/PS), and thermal activated-EC/PS for the treatment of two real produced water (PW) samples using iron electrodes were studied. To optimize and find out the effect of operating conditions on the different responses for EC and EC/PS, response surface methodology (RSM) was implemented. The results showed that EC process had considerable performance in the removal of H2S (96 %), oil and grease (O&G) (98–99 %), turbidity (91–97 %), phosphate phosphors (94 %), and heavy metals (92 %). EC/PS was introduced as an effective and a compact method for the removal of soluble hydrocarbons and nitrogen-ammonium (N-NH4+). The results indicated that at the current density of 35 A/m2, PS of 30 mM, reaction time of 30 min, N-NH4+ and chemical oxygen demand (COD) removal efficiency increased to 37 % and 71–94 %, respectively. To further increase the ammonia removal, EC/PS was integrated into thermal-PS activation at 65 °C, and the results showed that the ammonia removal by thermal/EC/PS reached about 69 %. According to gas chromatography/mass spectrometry (GC/MS), EC/PS was able to effectively eliminate most of the hydrocarbons. Moreover, a new kinetic model based on a novel algorithm and the main reactions occurring during EC/PS was developed to predict the COD removal efficiency, and the results indicated that it could predict COD removal efficiency with the acceptable accuracy. The estimated operating costs and energy consumption for EC/PS demonstrated that this process was more economical and efficient than other advanced oxidation processes (AOPs).

- **Keywords:** Produced water; Electro-oxidation; Electrocoagulation; Sulfate radicals; Saline wastewater

Xiaotong Xu, Hanmin Zhang, Tianyu Gao, Jiaheng Teng, Mengyang Lu. *Antibacterial thin film nanocomposite forward osmosis membranes produced by in-situ reduction of selenium nanoparticles*. Pages 403-412.

In this study, we present a facile method for the in-situ reduction of selenium nanoparticles (Se NPs) on a thin-film composite forward osmosis (FO) membrane. As an essential nutrient, Se is superior in terms of both low off-target toxicity and application potential. Given the superiority of Se, this study explored the application of Se NPs in the field of FO membrane separation and water treatment. In this study, Se NPs were evenly distributed on the polyamide layer of thin film nanocomposite (TFN) FO membranes and were found to significantly improve the hydrophilicity of the membrane surface and reduce the zeta potential value. Moreover, the water flux increased from 14.0 L m−2 h -1 (TFC FO) to 16.6 L m−2 h -1 (1 wt% Se TFN FO), while a slight increase in the reverse salt flux was observed. The diffusion inhibition zone tests revealed distinct antibacterial effects, and the bacteriostatic rate (BR) and live and dead cell staining tests showed a high BR (100 % of 1.5 wt% Se) of the Se NP-modified membranes on both gram-negative (Escherichia coli) and gram-positive bacteria (Staphylococcus aureus). Thus, Se NPs as antibacterial agents offer a new option for membrane functionalization and water treatment.

- **Keywords:** TFN FO membrane; In-situ reduction; Se nanoparticles; Antibacterial; Target toxicity

Xinhong Li, Luyao Zhang, Faisal Khan, Ziyue Han. *A data-driven corrosion prediction model to support digitization of subsea operations*. Pages 413-421.

Corrosion is an important factor leading to the failure of subsea process operations especially subsea crude oil pipelines. Developing a data-driven corrosion prediction model is urgently required by the digitization of subsea process system in the industry 4.0 environment, which is critical to improve the intelligent level of risk management of subsea process system. This paper proposed a new data-driven model based on hybrid

techniques to model corrosion degradation of subsea operations. The model is built integrating three data-driven methods: principal component analysis (PCA), artificial bee colony algorithm (ABC) and support vector regression (SVR). The developed model is tested on the corrosion rate prediction of subsea crude oil pipelines. This model can realize effective prediction of corrosion rate. In the proposed hybrid model, PCA is used to reduce the dimension of corrosion influencing factors. The obtained principal components are selected as the input variables of the model. The ABC algorithm is adopted to optimize the hyper-parameters of the SVR. The model is trained using fraction of the historical data; subsequently, the model performance is tested on the remaining set of the data. A case study demonstrates the feasibility and effectiveness of the proposed model. The model is compared with the four different models SVR, PCA-SVR, PCA-GA-SVR, PCA-PSO-SVR. The PCA-ABC-SVR model performed superior in terms of prediction accuracy and robustness of results (MAE = 7.10 %; RMSE = 9.19 %; R2 = 0.976). The proposed model will serve as a useful online tool to support safety and digitization of process system.

- **Keywords:** Corrosion rate prediction; Subsea crude oil pipelines; Principal component analysis; Artificial bee colony algorithm; Support vector regression

A. E. De Oliveira, V.G. Guerra. Electrostatic precipitation of nanoparticles and submicron particles: review of technological strategies. Pages 422-438.

Very small particles dispersed in the atmosphere display complex dynamics, due to their characteristics of Brownian motion and low sedimentation rate, while chemical and physical transformations in the air can lead to the formation of compounds that present greater risk. In this context, one of the most efficient gas-solid separators is the electrostatic precipitator (ESP), based on electrical charging of the particles and their attraction to collection electrodes. Therefore, this work summarizes the technological strategies employing ESPs to collect nanoparticles and submicron particles. The physical phenomena involved in particle charging and collection are described, together with discussion of the geometrical and operating differences between industrial-scale ESPs and small-scale devices. Studies and innovations involving strategies of design and operation are presented. Aspects of the electro-fluid dynamics in the device are described, as well as methods used to mitigate ozone production in this process.

- **Keywords:** Electrostatic precipitation; Nanoparticles; Submicron particles; Ultrafine particles; Pollution control; Gas cleaning

Hisham Al Baroudi, Kumar Patchigolla, Dhinesh Thanganadar, Kranthi Jonnalagadda. *Experimental study of accidental leakage behaviour of liquid CO2 under shipping conditions*. Pages 439-451.

CO2 shipping is a viable transport alternative when pipelines are impractical. Lack of experience in large-scale CO2 shipping projects implies uncertainty in selecting optimal cargo conditions and operational safety procedures. The risk of uncontrolled release of CO2 arises in case of mechanical failure of storage or cargo vessels, and a thorough understanding of the discharge phenomena, including the propensity for solid formation, is necessary to develop safety protocols. A refrigerated experimental setup is established in this study to investigate the release phenomena of liquid CO2 under shipping conditions. The rig features a dome-ended cylindrical pressure vessel, a discharge pipe section and a liquid nitrogen refrigeration system that enables conditioning near the triple point – at ~0.7 MPa, 223 K - and higher liquid pressures (~2.6 MPa, 263 K). Pressure, temperature and mass monitoring were considered to enable an extensive observation of the leakage behaviour under typical operation scenarios. Three different sets of experiments were considered to inform the designer in the selection of optimal process conditions, with low-pressure (0.7 – 0.94 MPa, 223–228 K), medium-pressure

(1.34–1.67 MPa, 234–245 K) and high-pressure tests (1.83–2.65 MPa, 249–259 K) demonstrating distinct behaviours relative to phase transitions, leakage duration and solidification of inventory.

- **Keywords:** GHG; CCUS; CO2 transport; CO2 shipping; Operational safety; Leakage

Beatriz Gimeno, Inmaculada Velasco, Javier Fernández, Sofía T. Blanco. *Evaluation of the simultaneous presence of SO2 and CO as impurities in the carbon capture and storage technology: CO2/SO2/CO cocapture*. Pages 452-463.

From the presented experimental data of two CO2-rich mixtures containing SO2 and CO as impurities of anthropogenic CO2, we evaluated the impact of the simultaneous presence of these impurities on the transport, injection and storage of carbon capture and storage (CCS) technology. We determined the density, vapor-liquid equilibrium and speed of sound of a cocapture mixture (non-purified captured flue gas) [CO2 + 4.93 mol% SO2 + 3.01 mol% CO] and a mixture representative of European emissions (purified) [CO2 + 0.09 mol% SO2 + 1.12 mol% CO], measured from 263 to 373 K and pressures up to 30 MPa for the density and up to 190 MPa for the speed of sound. Using our experimental results, we validated two extended versions of the equation of state for combustion gases (EOS-CG) and the perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (EoS). From the calculation of selected operational CCS parameters, we concluded that, in the cocapture mixture, SO2 overcomes or compensates for the negative effect of CO, and then this mixture could be a favorable fluid for CCS. The negative effect of CO predominates in the emissions mixture. Differences in the chemical reactivity due to the studied impurities were not considered.

- **Keywords:** CCS; Carbon dioxide; Sulphur dioxide; Carbon monoxide; Thermodynamic properties; Equations of state

Jiali Huo, Xiaoyang Luan, Yawen Gong, Zhi Wang, Juncheng Jiang, Bin Zhang. *Numerical study of bund overtopping phenomena after a catastrophic tank failure using the axisymmetric approach*. Pages 464-471.

Hazardous materials are stored in the large tanks in the industry, e.g., a single LNG tank can be as large as 230,000 m3. Therefore, a catastrophic tank failure can cause a disastrous incident. A secondary containment, such as a bund, is required by regulations to control the risk; however, the released liquid may overtop from the bund due to its high kinetic energy converted from potential energy. Computational Fluid Dynamic (CFD) is a proper tool for the bund overtopping study, but there has been significant discrepancy among previous CFD studies. This work developed 2D CFD models of bund overtopping using the axisymmetric approach. A screening study on several turbulence models was performed, and RNG k-ε Standard Wall Functions (RNG k-ε SWF1) and Large Eddy Simulation WALE (LES WALE) were selected for a detailed comparison in terms of overtopping fraction and flow dynamic behaviour. Both RNG k-ε and LES models were systematically validated against experimental data, and the results indicate that LES model is slightly better than RNG k-ε model, and both models are acceptable based on the criteria of statistical performance measures.

- **Keywords:** Storage tank; Catastrophic failure; Secondary containment; Bund overtopping; CFD

Mohammad Zaid Kamil, Mohammed Taleb-Berrouane, Faisal Khan, Paul Amyotte. *Data-driven operational failure likelihood model for microbiologically influenced corrosion*. Pages 472-485.

Corrosion is a threat to asset integrity, with engineering challenges and economic burdens. Since the last decade, microbiologically influenced corrosion (MIC) began to be recognized among corrosion professionals as a severe corrosion form. It is challenging to detect and predict MIC due to the complex behaviour of microorganisms. The current MIC risk assessment models define the dependencies of parameters with their synergic interactions. A data-driven approach is needed to utilize available operational and microbiological data and learn as the data changes. The model proposed in this study is used to strengthen the variables' correlation and their features to assess MIC likelihood. It can integrate available field and laboratory data into a Learning-based Bayesian network (LBN) model. The model minimizes current research gap and has the advantage of adapting to changes in process operation. It is based on an advanced Bayesian learning algorithm, which develops topology of the Bayesian network (BN) from the input data and its parameters. This paper focuses on the development of the LBN model that utilizes available MIC data for likelihood estimation. The model is benchmarked and validated using data reported in the public domain. The application of the model is demonstrated on the processing facility on a Floating, Production, Storage and Offloading (FPSO). The topology and parameter estimation will update as data changes/improve to capture the system behaviour to assess MIC likelihood, which helps in decision-making to control and mitigate MIC threats.

- **Keywords:** Corrosion; Microbiologically influenced corrosion (MIC); Learning-based bayesian network (LBN); Bayesian learning; Floating; Production; Storage and offloading (FPSO)

Mohammed Bougofa, Mohammed Taleb-Berrouane, Abderraouf Bouafia, Amin Baziz, Rabeh Kharzi, Ahmed Bellaouar. *Dynamic availability analysis using dynamic Bayesian and evidential networks*. Pages 486-499.

The probabilistic modelling is widely used in engineering practices, especially for assessing the safety and reliability of complex systems. Dynamic evidential network (DEN) can efficiently deal with epistemic uncertainty based on Dempster-Shafer theory. This work proposes an extended discrete-time DEN model along with an extensive review of its applications in engineering. The proposed model combines the Dempster-Shafer theory, used for handling epistemic uncertainty across a new state-space reconstruction of components, and the dynamic Bayesian network is used for multi-state system reliability. The model application is demonstrated on a real case study from the aviation field. The application quantifies reliability and availability parameters that help to prioritize maintenance activities and avoid failures of complex redundant systems. The proposed model can serve as a tool to assess the reliability and availability of industrial systems suffering from parameter uncertainty and common cause failures.

- **Keywords:** Evidence theory; Evidential network; Common cause failure; Parameter uncertainty; Dempster-Shafer theory; Availability

Hassan E. Gomaa, Abdullah A. Alotaibi, Fatma. A. Gomaa, Elham Bajuayfir, Ashfaq Ahmad, Khalid M. Alotaibi. *Integrated ion exchange-based system for nitrate and sulfate removal from water of different matrices: Analysis and optimization using response surface methodology and Taguchi experimental design techniques.* Pages 500-517.

Although sequestering nitrate by anion exchange resins (AERs) is a proven and well-established technology, many process problems and challenges still exist, such as interference, nitrate dumping, total dissolved solids (TDS) limitations, brine waste disposal, etc. An engineered-integrated approach was devised and assessed to mitigate such limitations. The overall process optimization was based on screening, analyzing, and optimizing each respective step. A front-end sulfate removal step was suggested, evaluated, which yielded removal efficiencies >95%. Back-end options were also introduced, including reduced brine and brine wastes, recycling possibility, and usage as mixed-fertilizer with a NO3/Cl ratio of 0.65 as confirmed by mass balance calculations. Taguchi robust designs (TRD), Box-Behnken Designs (BBD), and central composite design (CCD) experimental design methods were used, enabling information mining from a minimum number of experiments. A one-factor-at-a-time strategy was applied and the regeneration process was optimized using TRD. Response analysis and regression revealed that acid concentration and volume are the most influential factors. Selectivity order was determined as SO42-->Cl−>HCO3− according to their relative coefficients of the BBD and CCD regression models. Field trials confirmed the robustness and viability of the proposed integrated approach. A process flow diagram was devised. Merits of the proposed system include: a) possible resolution of sulfate competition and nitrate dumping, b) elimination of brine waste problems, c) tolerate higher TDS levels than ever possible for AERs, d) improved economics, e) improved process robustness, f) mitigate the corrosiveness of produced water, and g) fulfilling zero liquid discharge criteria.

- **Keywords:** Nitrate and sulfate removal; Ion exchange; Taguchi design; Water process engineering; ZLD

Jiaxi Jiang, Sherub Phuntsho, Nirenkumar Pathak, Qilin Wang, Jaeweon Cho, Ho Kyong Shon. *Critical flux on a submerged membrane bioreactor for nitrification of source separated urine*. Pages 518-526.

Membrane fouling is the biggest challenge in membrane based technology operation. Studies on critical flux mainly focused on membrane bioreactor for municipal wastewater and/or greywater treatment, which can significantly differ from the ultrafiltration membrane bioreactor (UF-MBRs) to treat source separated urine. In this work, the inhibitory factors on nitrifying bacteria activity were investigated for fast acclimation of nitrifying bacteria with high ammonium concentration and optimization of a high-rate partial nitrification MBR. The maximum nitrification rate of 447 ± 50 mgN L−1 d−1 was achieved when concentration of ammonia in feed urine is approximately 4006.3 ± 225.8 mg N L−1 by maintaining desired pH around 6.2 and FA concentrations below 0.5 mgL−1. Furthermore, for the first time, the impact of different operational and filtration conditions (i.e. aeration intensity, filtration method, imposed flux, intermittent relaxation, biomass concentration) on the reversibility of membrane fouling was carried out for enhancement of membrane flux and fouling mitigation. Fouling mechanisms for minor irreversible fouling observed under sub-critical condition were pore blocking and polarization. To mitigate membrane fouling, the UF module with effective membrane surface area of 0.02 m2 is recommended to be operated at the aeration intensity of 0.4 m3 h−1, intermittent relaxation of 15 min, biomass concentration of 3.5 g L−1.

- **Keywords:** Submerged ultrafiltration membrane bioreactor (UF-MBR); Critical flux; Critical flux for irreversibility; Fouling reversibility; Source separated urine; Improved flux-step method

Xiao-Qiao Zhao, Wen-Qian Wu, Hua-bo Li, Zi-Chao Guo, Wang-Hua Chen, Li-Ping Chen. *Thermal hazards of benzaldehyde oxime: Based on decomposition products and kinetics analysis by adiabatic calorimeter*. Pages 527-536.

As a self-reactive substance, benzaldehyde oxime (BO) is prone to a highly exothermic runaway reaction and thermal hazard analysis and the reaction kinetics calculation of BO have great significance. In this work, the decomposition products of BO in nitrogen atmosphere were identified by GC–MS and HPLC techniques. The impact of the decomposition products on the decomposition behaviors of BO were analyzed by comparison of the ARC test results of pure BO and mixture of BO and decomposition products. It was found that N-benzylidene benzylamine was the intermediate decomposition product and benzoic acid, benzamide, N-benzyl benzamide, and 2,4,5-triphenylimidazole were the final products of BO. A two-step continuous autocatalytic reaction model was established to depict the decomposition process of BO. The kinetic parameters of the model were calculated by applying the nonlinear optimization method. Finally, thermal behaviors under different process temperature were predicted based on the kinetic model, and the time to maximum rate (TMRad) was predicted as 112.04 °C under 24 h, and 122.19 °C of 8 h, which offer crucial safety information to optimize the safety conditions of BO during usage, storage and transportation, which minimizes the industrial disasters.

- **Keywords:** Benzaldehyde oxime; Thermal hazards; ARC; Product analysis; Kinetics-based simulation