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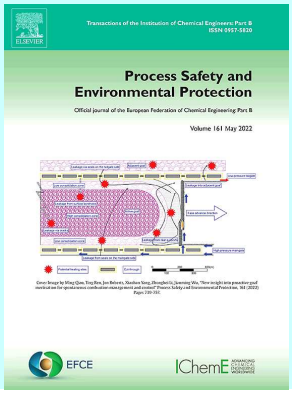


**Shixiang Liu, Xiaolei Zhang, Xu Fang, Longhua Hu. *Experimental study on tilting behavior and blow out of dual tandem jet flames under cross wind*. Pages 1-9.**

Fire hazards in outdoor environmental conditions cause huge damage to process safety in fuel transportation and pipeline leakage. Few literatures are reported about the combustion behaviors and instability characteristics of dual jet flames under cross wind, which are important to risk assessment and manufacturing design. In this work, a series of propane fire source with nozzle diameters of 3 mm, 4 mm and 5 mm are designed for different nozzle separation distances under cross wind. Results showed the tilt angle of rear jet flame was smaller than front jet flame due to the vitiated effective wind towards the rear jet flame by the blockage of the front jet flame. Furthermore, it's found that the blow-out cross wind velocity of the rear jet flame is smaller than that of the corresponding single jet flame. The combustion of the front jet flame will restrict the rear jet flame to a certain extent. Finally, dimensional analysis and correlations are established, where the blow-out cross wind velocity of rear jet flame as well as that of the single jet flame can be well represented by Froude number. These new observations and correlation are helpful for further understanding combustion behaviors of dual tandem jet flames under cross wind.

- **Keywords:** Dual tandem jet flame; Separation distance; Cross wind; Tilt angle; Blow out

**Qiaona Xie, Haifeng Zhuang, Ruting Liang, Yufei Zhao, Xiaoying Zhan, Haojie Tang, Hao Wu. *Potential mechanism of enhanced anaerobic degradation of high concentration phenol-containing wastewater by hazardous waste fly ash with high iron content: Direct interspecies electron transport pathway*. Pages 10-19.**

Micron-grade high iron-containing fly ash (MHIFA) - a processed hazardous waste containing Fe3O4—was added to an up-flow anaerobic sludge blanket reactor to improve the removal performance of high concentration phenol-containing wastewater. The chemical oxygen demand and total phenol removal efficiency with MHIFA were 72.13%

and 81.83%, respectively. Moreover, MHIFA addition increased the contents of coenzyme F420 and extracellular polymeric substances, as well as higher electron transport system activity in activated sludge. Additionally, microbial community analysis revealed that the total methanogens contents increased at genera level, producing an increase in methane production, while enriched Geobacter along with archaea Methanothrix might collaborate in direct interspecies electron transfer (DIET) by MHIFA stimulation, promoting the effect of phenolic compound fermentation. Finally, this technology allows for resource utilization of hazardous waste and enhances anaerobic degradation of toxic and refractory pollutants.


- **Keywords:** MHIFA; Phenol-containing wastewater; Geobacter; Direct interspecies electron transfer


### Xing Guo, Qiang Feng, Dongming Fan, Zili Wang, Yi Ren, Bo Sun, Dezhen Yang. *An agent-based dynamic reliability modeling method for multistate systems considering fault propagation: A case study on subsea Christmas trees*. Pages 20-33.


The fault propagation of multistate systems (MSSs) with various operational modes is a critical factor affecting the reliability and safety of systems. However, traditional methods have difficulty describing the influence of function transitions and multiple faults of components on fault propagation, and are inapplicable for accurately evaluating the dynamic reliability of MSSs. To solve these issues, an agent-based method is developed to evaluate the dynamic reliability of MSSs. This study proposes a reliability modeling framework that consists of a management agent and several system agents. Combined with different agents, two types of models are established to describe the logical relationships among components. Moreover, Monte Carlo simulation is used to evaluate the dynamic reliability of MSSs, and a visual failure paths analysis method is proposed to inhibit potential risk. The LH4–1 horizontal Christmas tree is used to verify the effectiveness of proposed method. Under the designed working condition, the dynamic reliability curve of system with three operational modes and the visual failure paths including 15-node are obtained. By comparing the influence of failure rates, it is found that the production choke valve, flowlines, tree cap and MEG chemical control valve have a great impact on the system reliability.



- **Keywords:** Multistate system; Reliability modeling; Dynamic reliability; Agent-based model; Subsea Christmas tree


### Yan Yu, Chengwei Xu, Jun Zhang, Chao Fu. *Effects of coal-fired flue gas composition on condensational growth by water vapor for fine SiO2 particles*. Pages 34-41.


The effects of main components of coal-fired flue gas after desulfurization on the supersaturated environment achievement and condensational growth for SiO2 particles by water vapor were analyzed. The predicted results demonstrate that the variation of CO2 content has the greatest impact on the heat and mass transfer in the flue gas. Moreover, it is unfavorable for heat and mass transfer when the CO2 content increased. Thus, the improvement of CO2 content has great advantage of achieving supersaturated environment by the method of heating the gas flow. Similarly, the component of SO2 also has the negative influence on the heat and mass transfer when its content increased. For the improvement of O2 content, it is slightly beneficial for the thermal and mass diffusion coefficient of water vapor. Additionally, the process of thermal diffusion will be weakened while the mass diffusion will be facilitated when the amount of water vapor enhanced. Meanwhile, the experimental results indicate that particle growth is significantly improved with the increase of CO2 content by the supersaturation achieving method of heating gas flow. Nevertheless, it has slightly negative effect on the particle

enlargement by cooling the gas flow when the CO2 content promoted. It can be seen that the influence of coal-fired flue gas composition on the condensational growth by water vapor is different by different supersaturation achieving methods.

- **Keywords:** Fine particulate matters; Flue gas composition; Heterogeneous condensation; Supersaturated environment; Thermal and mass diffusion

### Lei Zhu, Zhou Shi, Lin Deng, Jing Chen, Haojie Zhang. *Fabrication of Epigallocatechin-3-gallate (EGCG) functionalized Mn3O4 for enhanced degradation of carbamazepine with peroxymonosulfate activation*. Pages 42-54.

Peroxymonosulfate activation via heterogeneous catalyst was broadly applied for the treatment of PPCPs. In this work, a novel material of Epigallocatechin-3-gallate (EGCG) fuctionalized Mn3O4 nano-octahedra (E@MO) was synthesized and utilized for the degradation of carbamazepine. Various technologies such as X-ray diffraction, Fourier transform-infrared spectroscopy, Scanning electron microscope, Transmission electron microscope, Brunauer-Emmett-Teller and X-ray photoelectron spectroscopy were employed for the characterization of the as-synthesized catalyst. The results depicted that under the conditions of CBZ concentration 5 mg/L, PMS concentration 1 mM, catalyst dosage 0.2 g/L, initial pH 5.8 and 25 °C, the targeted pollutant could be totally degraded in 60 min with a rate constant of 0.0622 min−1. When temperature raised to 45 °C, CBZ was removed completely in 20 min and the rate constant (0.1668 min−1) was 2.59 times than that of 25 °C, implying the degradation process was an endothermic reaction. Scavenging experiments and EPR analysis confirmed the main reactive oxygen species generated in the reaction were sulfate radical (SO4•) and hydroxyl radical (•OH), while SO4• serviced as the leading role. Due to the reduction property of EGCG, compared with bare Mn3O4, the CBZ degradation was markably enhanced and the degradation reaction were accurately matched with the pseudo first-order kinetics equation. The possible twelve intermediates produced in the decomposition of CBZ were identified by HPLC-MS/MS, their ecotoxicity were evaluated and compared by ECOSAR model. Together with the consequences, the degradation mechanism of CBZ in the E@MO/PMS system was propounded.

- **Keywords:** EGCG; Mn3O4; Peroxymonosulfate; Carbamazepine; AOPs

### Srinivas Sivaraman, S.M. Tauseef, N.A. Siddiqui. *Investigative and probabilistic perspective of the accidental release of styrene: a case study in Vizag, India*. Pages 55-69.

In addition to revealing the cracks in global health care, emergency preparedness, and response systems, COVID-19 also exposed the lack of capacity to run chemical plants safely under such conditions. On 7th May 2020, self-polymerization runaway reaction from an atmospheric storage tank in a polymer facility triggered the release of styrene to the atmosphere, resulting in 12 fatalities and hospitalization of more than 1000 individuals. A similar incident had happened 35 years back at Bhopal involving the release of methyl isocyanate resulting in one of the deadliest process safety incidents to date. Therefore, it is very important to understand the causal factors so that such high-risk incidents can be prevented in future. This paper presents a comprehensive investigative study of styrene gas leak at Vizag with special emphasis on probabilistic risk analysis of the loss of containment. Hazard perception study was performed to understand the possible hazardous scenarios in bulk styrene storage facilities for preventing such catastrophic recurrences. Energy barrier analysis was performed to study the inadequacy of pro-active and reactive barriers with respect to the accident case study. The analysis also considers the escalation factors resulting from extremities of COVID-19 lockdown. The self-polymerization reaction that resulted in toxic styrene

dispersion was preventable owing to the advancements in safety engineering and loss prevention since Bhopal Gas Tragedy (1984). Based on the investigative analysis, it can be pointed out that this accident would have occurred even in the absence of COVID-19 restrictions, mainly due to negligence and complacency shown towards safety by the company's management.


- **Keywords:** Loss of containment; Accident analysis; Probabilistic risk assessment; Energy barrier model; Lessons learnt


**Xiaoli Dai, Jing Lv, Wenxia Wei, Shaohui Guo. *Bioremediation of heavy oil contaminated intertidal zones by immobilized bacterial consortium*. Pages 70-78.**


Heavy oil contamination adversely affects on the intertidal ecological environment and human health. In this study, immobilized bacterial consortium was used in remediating intertidal zones contaminated with heavy oil, and its effectiveness was investigated in simulation experiment pools constructed in the coastal areas. After 100 days, the heavy oil degradation efficiency of immobilized bacterial consortium was 52.99%, which was 13.57% and 30.61% higher than that of biostimulation and natural attenuation, respectively. The immobilized bacterial consortium significantly increased the microbial degradation activity, heavy oil-degrading microbial count, and heavy oil degradation efficiency. Gas Chromatography–Mass Spectrometry results revealed that the biodegradation efficiency of C15–C35 n-alkanes and 2–5-ring polycyclic aromatic hydrocarbons was 25.98–95.80% and 58.93–97.97%, respectively. Microbial community structural analysis showed that Acinetobacter sp. and Bacillus sp. were prominently involved in heavy oil biodegradation. Furthermore, the immobilized bacterial consortium not only resisted the invasion of adverse intertidal environment and promoted the biodegradation of heavy oil pollutants in sediments but also effectively increased the competitiveness between the indigenous oil-degrading microorganisms and other microorganisms. This study can be a promising approach to remediate heavy oil contaminated intertidal zone.



- **Keywords:** Heavy oil; Intertidal zones; Bioremediation; Immobilized bacterial consortium


**Lu Wang, Ting Li, Liangliang Tao, Hanwu Lei, Peiyong Ma, Jian Liu. *A novel copper-doped porous carbon nanospheres film prepared by one-step ultrasonic spray pyrolytic of sugar for photocatalytic degradation of methyl orange*. Pages 79-86.**


Copper-doped porous carbon nanospheres film (Cu@PCNF) was prepared via one-step ultrasonic spray pyrolysis (USP) for photocatalytic degradation of methyl orange (MO). The photocatalytic degradation rate reached 80% after 4 h under sunlight, and kinetic simulation results showed that the degradation reaction was a first-order reaction. Furthermore, the degradation rate did not decrease significantly after eight experiment cycles, which indicated that the film had good reusability and durability. This film synthesis technology provided a simple and effective strategy for improving the photocatalytic performance of contaminant treatment materials.



- **Keywords:** Porous carbon; Ultrasonic spray pyrolysis; Cuprous oxide; Photocatalysis; Methyl orange


**Yijuan Tian, Xuejun Quan, Gang Li, Xiaoyu Tang, Xianfeng Qin, Haifeng Wu, Kui Zeng, Zhanghao Jiang. *A cleaner method for preparation of chromium oxide from chromite ore*. Pages 87-97.**

To establish a cleaner production technology of chromium salt, the pressurized leaching process of chromite ore in 60 wt% NaOH solution, subsequent separation of a chromium salt from the leached solution and Cr2O3 preparation from the intermediate product BaCrO4 were systematically investigated, and a new highly efficient and economical process for the production of Cr2O3 from chromite ore was established. The results showed that the decomposition of chromate ore could be significantly improved by increasing the temperature, and the Cr leaching rate reached 99% at 240 °C for 4 h. Meanwhile, the leaching process was controlled by surface chemical reactions with activation energy (Ea) of 34.3051 kJ/mol and a pre-exponential factor (A) of 6.9560. In the leached liquor, Na2CrO4 was transformed into BaCrO4 through its reaction with Ba(OH)2, Cr separation efficiency could reach as high as 89% in the undiluted leached liquor, while the separated alkali liquor could be effectively recycled for the leaching of chromite ore. Ultimately, a new method for the preparation of Cr2O3 from the intermediate product BaCrO4 was presented by the dissolution and reduction of BaCrO4 with HCl-CH3CH2OH as the reactant. The new cleaner process for Cr2O3 preparation from chromite ore provides an attractive alternative to upgrading the current chromate salt production processes.

- **Keywords:** Chromite ore; Oxidative leaching; Chromate salt separation; Cr2O3; Clean process

### **Mengxi Yu, Hans Pasman, Madhav Erraguntla, Noor Quddus, Costas Kravaris. *A framework to identify and respond to weak signals of disastrous process incidents based on FRAM and machine learning techniques*. Pages 98-114.**

Most incidents in complex systems such as process plants are not-chance events and weak signals emerge for a long time before incidents occur. It is necessary to identify and respond to the weak signals as early as possible for preventing incidents. However, in the era of Industry 4.0, recognizing weak signals from the abundance of data is challenging. Since the terminology "weak signal" was not precisely defined, the study first proposed a formal definition of "weak signal" and discussed its characteristics. Additionally, a framework was developed to address the challenges of observing, evaluating, and responding to weak signals in complex systems. The framework first utilized Function Resonance Analysis Method (FRAM) to determine the information to be collected for observing weak signals. Then, the relevance of weak signals and the corresponding responses were evaluated by utilizing Balanced Random Forest (BRF), Weighted Random Forest (WRF) and Decision Tree (DT) classification models. The case study of a hypothetical batch process showed great potentials for applying the framework in real operations. Based on the potential weak signals that were indicated by FRAM, probabilities of temperature deviations in the process were predicted with high accuracy by the optimal BRF model. Underlying weak signals and the corresponding responses to reduce the probabilities were identified from the DT.

- **Keywords:** Complex system; Preventive Safety; Weak signals; Machine learning; Probability calibration

### **Jianping Zhang, Jiaqi Wang, Zexin Jiang, Dacheng Xu. *Trapping PM2.5 particles from electrostatic precipitator equipped with magnetic field under different gas velocities*. Pages 115-122.**

The aim of this work is to investigate the effects of magnetic field and ionic wind on the ability of a wire-plate electrostatic precipitator (ESP) to trap fine particles. A theoretical model of multi-field coupling between gas flow field, particle dynamic field and electromagnetic field was established, and a grid model was built by GAMBIT software. The collection efficiency under different gas velocities was calculated in FLUENT software

where the electric field force and the magnetic field force were introduced by User Defined Function (UDF). The numerical results indicate that both ionic wind and applied magnetic field can effectively improve the PM2.5 collection efficiency in a wire-plate ESP, and the smaller the particle size, the more obvious the improving effects are. With the increase of gas velocity, PM2.5 collection efficiency has a nonlinear declining trend, but the contribution of ionic wind or magnetic field to the collection efficiency increases. The trapping performance of the wire-plate ESP under the combined action of the two factors is better than that of considering one of them separately. The research results can open up a new design idea and direction for the performance upgrading of the wire-plate ESP.


- **Keywords:** Wire-plate ESP; PM2.5; Magnetic field; Ionic wind; Multi-field coupling; Gas velocity


**Juwon Lee, Yuchan Ahn, Hyungtae Cho, Junghwan Kim. *Economic performance assessment of elemental sulfur recovery with carbonate melt desulfurization process*. Pages 123-133.**

This study develops an elemental sulfur recovery (ESR) process from sulfur dioxide (SO2) as a hazardous material removed from flue gas emitted at thermal coal-fired power plants with a carbonate melt flue gas desulfurization (CMFGD) process. The carbonyl sulfide (COS) generated as a byproduct after removing SO2 from flue gas using carbonate melt in the CMFDG is utilized as a resource to produce elemental sulfur by applying the hydrolysis and Claus processes in the ESR process. In addition, to increase energy independence in the integrated CMFGD-ESR process, heat integration was applied by introducing new heat exchanger networks that utilize the waste heat in the proposed process. The levelized cost of the integrated CMFGD-ESR process was determined to be US$ 811 per ton SO2 removed; from this result, the proposed process to remove hazardous material from flue gas emitted at thermal coal-fired power plants is economically benign compared to conventional SO2 removal processes (US$ 500 ~ US$ 1200 per ton SO2 removed), which use limestone as the raw material.


- **Keywords:** Carbonate melt; Flue gas desulfurization; Elemental sulfur recovery; Claus process; Economic feasibility


**Kai Wang, Long Wang, Yang Ju, Huzi Dong, Wei Zhao, Changang Du, Yangyang Guo, Zhen Lou, Han Gao. *Numerical study on the mechanism of air leakage in drainage boreholes: A fully coupled gas-air flow model considering elastic-plastic deformation of coal and its validation*. Pages 134-145.**

Air leakage caused by mining-induced fractures around the borehole and roadway greatly affects the effect of underground gas drainage. Therefore, the study of the air leakage model considering three-dimensional stress and coal elastic-plastic deformation is of great significance to prevent air leakage. In this work, a model of air leakage outside borehole in mining-disturbed coal seam including a fully coupled gas-air flow and coal mechanics model and a mining-induced damage permeability model was developed and verified. The model was used to study the gas-air migration law and air leakage mechanism during gas drainage, and the influence of key parameters including initial permeability and sealing depth on gas drainage effect was analyzed. The results show: (1) The model can be used to characterize the air leakage of pre-drainage boreholes in mining-disturbed coal seams. (2) The gas and air pressure in the severe mining disturbance area rapidly decreased and increased in a short time. (3) Increasing the initial permeability and sealing depth will promote the gas flow in the borehole in the early stage, but the gas concentration will be reduced. The research results provide a scientific theoretical basis for improving the gas drainage effect and ensuring mining safety.

- **Keywords:** Gas drainage; Air leakage; Strain-softening; Permeability; Sealing depth

**Xingmin Cui, Mingguang Zhang, Wenjie Pan. *Dynamic probability analysis on accident chain of atmospheric tank farm based on Bayesian network*. Pages 146-158.**

Due to massive flammable chemical materials and dense layout, domino accident chain always occurs in major accidents of atmospheric storage tank farm. In this paper, 136 domino effect accidents of atmospheric tanks are analyzed to achieve relative probability by ETA method. Based on accident probability, an analysis model is proposed to define the most likely accident chain and the key tank in the atmospheric tank farm. To get the real accident scenario, the method adopts the heat radiation model of pool fire under the fire extinguishing conditions. Combined with the dynamic Bayesian network, the escalation model of accident chain is established to figure out the dynamic probability of the tank under the condition of fire extinguishing. Finally, an example is used to verify the feasibility of the method. It is of great theoretical significance and application value for the treatment of domino accident in atmospheric tank farm.

- **Keywords:** Atmospheric tank; Domino accident chain; Escalation probability model; Dynamic Bayesian network

**Mohammad Yazdi, Faisal Khan, Rouzbeh Abbassi. *Operational subsea pipeline assessment affected by multiple defects of microbiologically influenced corrosion*. Pages 159-171.**

This paper presents a systematic approach to evaluate the time interval of optimal maintenance strategy for the subsea process system influenced by Microbiological Influenced Corrosion (MIC) within multiple defects. The proposed method incorporates the non-homogeneous Poisson, homogeneous gamma, and non-homogeneous Markov processes for modeling the generation of multiple defects, the average pit depth growth, and maximum pit depth, respectively. The maintenance strategy comprises industrial procedure, probability of failure detection, errors sizing in-line inspection tools, management actions costs, and failure cost. The developed framework simulates maintenance strategies considering time interval, cost, probability of detection, average pit depth, and maximum pit depth and identifies the optimal strategy. The practical application is demonstrated in a North Sea subsea pipeline system under MIC's influence. This work assists decision-makers in selecting the optimal conditioned-based maintenance strategy for the processing system. While the application is demonstrated to subsea process systems under MIC influence, the developed approach is equally applicable to other process systems.

- **Keywords:** MIC management; Reliability-based maintenance; Markov process; Condition Modelling

**Junyuan Guo, Chongrui Yuan, Ziyu Zhao, Qianlan He, Hengbing Zhou, Ming Wen. *Soil washing by biodegradable GLDA and PASP: Effects on metals removal efficiency, distribution, leachability, bioaccessibility, environmental risk and soil properties*. Pages 172-180.**

Washing is one of the most practical remediation methods for heavy metals contaminated soil, however, conventional washing agents always cause soil acidification and salinization and bring about other negative impacts on soil microbes and plants. This study selected glutamate-N,N-diacetic (GLDA) and polyaspartic (PASP) as biodegradable chelators to remove Cd, Pb and Zn from contaminated farmland soil. The residual metals' leachability, bioaccessibility, environmental risk and the properties of the soil were

investigated after the polluted soil was washed with GLDA and PASP. Results showed that 93.8% of Cd, 87.9% of Pb and 91.9% of Zn were washed out when the concentration of GLDA was 50 mmol/L, pH was 5.5, S/L ratio was 1:10 and contact time was 90 min. Meanwhile, compared with the original soil, the leachability and bioaccessibility of the residual metals were decreased and the stability was increased after washing by GLDA or PASP. The environmental risks of metals were decreased as well by decreasing their bioaccessible concentrations. Moreover, the activity of the soil enzyme was improved after leaching. To sum up, this study provided a theoretical and scientific basis for the treatment of soil heavy metals pollution with biodegradable chelator.

- **Keywords:** Soil washing; Biodegradable washing agent; GLDA; PASP; Soil properties; Heavy metals

### Yuanyuan Shen, Zihao Su, Qing Zhao, Rongli Shan, Zhaoyou Zhu, Peizhe Cui, Yinglong Wang. *Molecular simulation and optimization of extractive distillation for separation of dimethyl carbonate and methanol*. Pages 181-188.

Dimethyl carbonate, an important green solvent, has garnered substantial attention in recent years. The routes for dimethyl carbonate synthesis include transesterification, alcoholation of urea by methanol, and oxidative carbonylation of alcohols. The transesterification process accounts for the largest proportion of dimethyl carbonate synthesis because it affords a high conversion rate of the raw materials, easy separation of the products, and is the most mature process. The azeotrope of dimethyl carbonate and methanol in the top of the columns used for preparing dimethyl carbonate by transesterification needs to be further separated. Herein, the optimal ionic liquid ([BMIM][OTF]) for the separation of dimethyl carbonate and methanol via extractive distillation was determined by applying a molecular dynamics simulation algorithm and utilized in the separation process. As an efficient and green energy-saving process, pervaporation-assisted extractive distillation was further evaluated for the separation of dimethyl carbonate and methanol. The results showed that the pervaporation-assisted extractive distillation process offers economic benefits and has less environmental impact, and its total annual cost is 17.28% lower than that of the common extractive distillation process. Environmental analysis showed that carbon dioxide emissions, sulfur dioxide emissions, and nitric oxide emissions were reduced by 49.09% with this process. Therefore, this research has important guiding significance for the realization of the high-efficiency, energy-saving, and green separation of dimethyl carbonate and methanol in industries.

- **Keywords:** Dimethyl carbonate; Extractive distillation; Pervaporation; Economic; Environmental

### Gülsev Soysüren, Ayşe Gül Yetgin, Özgür Arar, Müşerref Arda. *Removal of manganese (II) from aqueous solution by ionic liquid impregnated polymeric sorbent and electrodeionization (EDI) techniques*. Pages 189-198.

Manganese is an element that is essential for the proper functioning of humans and animals, as it is needed for the functioning of many cellular enzymes. However, overexposure to this metal can be toxic to many organ systems and at various stages of life. In this work, ionic liquid impregnated polymeric sorbent (ILIS) and electrodeionization (EDI) processes were used to remove manganese (Mn2+) from aqueous solutions. The removal of Mn2+ by ILIS is pH dependent and maximum removal is achieved at pH 9. The sorption of Mn2+ on ILIS reached equilibrium in 20 min. For Mn2+ removal by EDI, the applied potential, feed flow rate and H2SO4 concentration in the electrode compartment were optimized. When the applied potential and feed flow rate were increased, the Mn2+ concentration in the feed solution decreased. Varying the

H2SO4 concentration in the electrode compartment did not result in differences in the removal rate. The largest calculated flux for Mn2+ is 6.92 × 10−5 mol/m2s, and the mass transfer coefficient is 8.16 × 10−4 m/s. In the last phase of the experiment, ILIS-EDI hybrid techniques were used for the removal of Mn2+. In this case, more than 99.9% was removed from the solution.


- **Keywords:** Hyphenated technique; Ionic liquid; Electrodeionization; Manganese; Water treatment


**Omid Bahadorizadeh, Mohammad Amin Sobati, Shahin Shahnazari. *Emission characteristics of a semi-industrial boiler fueled by waste cooking oil biodiesel containing different metal oxide nanoparticles*. Pages 199-209.**

In the present study, the emission of a semi-industrial boiler has been investigated using the waste cooking oil biodiesel (WCO) blended with the different nanoparticles, including CeO2, Al2O3, and Co3O4. The nanoparticles were blended to the WCO biodiesel in three different concentrations (25, 50, and 100 ppmw), considering the different combinations of single, binary, and ternary compounds. The results confirmed that there is a synergistic effect by the addition of CeO2, and Co3O4. It was also found that the application of B-Ce-Co-Al50 fuel sample (WCO biodiesel containing 50 ppm cerium oxide, cobalt oxide, and aluminum oxide) leads to the lowest value of CO emission. The CO emission for this fuel sample was 74%, and 43% lower compared to the neat diesel, and WCO biodiesel, respectively. The lowest flame temperature and the lowest NOX emission was observed for B-Ce-Co100 fuel sample (WCO biodiesel containing 100 ppm cerium oxide and cobalt oxide). The NOX emission for this fuel sample was 10%, and 39% lower compared to the diesel, and the WCO biodiesel, respectively.


- **Keywords:** Waste cooking oil (WCO); Biodiesel; Emission; Nanoparticle; Combustion; Semi-industrial boiler


**Yunbei Li, Zexu Chen, Hailong Li, Qianjing Yao, Yi Wei, Xin Wang, Ninghao Wang, Xinyu Cao, Mengyu Zheng, Jinghua Lv, Zhensheng Guo, Jishao Jiang. *Improving dewaterability of sewage sludge by inoculating acidified sludge and Fe2+: Performance and mechanisms*. Pages 210-220.**

Bioleaching is considered to be an economical and environmentally friendly strategy for sewage sludge (SS) dewatering and heavy metal removal. Acidified sludge (AS), exhibiting strong Fe2+ oxidation capacity, was obtained by repeatedly domesticating sewage sludge with Fe2+, and was treated as a novel inoculum to enhance SS dewaterability during the bioleaching process. AS addition accelerated Fe2+ oxidation and reduced the pH from 7.57 to 2.81 because of bio-acidification and bio-oxidation. After conditioning for 48 h, the SS dewaterability improved in Fe2+-treated and AS conditioned samples; the capillary suction time (CST) and specific resistance to filtration (SRF) decreased from 157.6 s and 12.5 × 1012 m/kg of raw sludge to 40.9 s and 0.53 × 1012 m/kg. Compared with the raw sludge, the total protein content in tightly bound extracellular polymeric substances (TB-EPS) decreased by 82.5% after AS and Fe2+ treatments, while it decreased by 9.69% after treatment with only Fe2+. Three-dimensional fluorescence spectroscopy showed that the decomposition of aromatic proteins, tryptophan-like proteins, and soluble microbial products in TB-EPS contributed in improving SS dewaterability. The results of microbial diversity revealed that in addition to bioleaching microorganism Acidithiobacillus playing an important role, other acid-tolerant microorganisms such as Acidocella, Thiomonas, and Metallibacterium also contribute in improving the SS dewatering performance. The symbiotic association of the

above microorganisms reduced the environmental pH and protein concentration, changed the protein composition, thus promoting the release of the bound water contained in SS.

- **Keywords:** Sludge conditioning; Bioleaching; Dewatering; Extracellular polymeric substances; Microbial community

### Xuanze He, Jun Fang, Yue Zhang, Luyao Zhao. *Experimental study of flame spread transition from chemistry to heat transfer controlled regime at sub-atmospheric pressure: The effect of sample width*. Pages 221-230.

Understanding the flame spread rate (FSR) is controlled by either chemistry or heat transfer is important for industrial process safety. In this study, we study the effect of width on flame spread transition from chemical to thermal regime at sub-atmospheric pressure using thin paper sample with widths from 10 mm to 90 mm. Results show that the transition boundary can be identified using not only reported FSR but also the flame image or radiation, as each of them has significantly different characteristics in different regimes. We find that the orientation significantly affects the flame spread in the thermal regime but has negligible influence in chemical regime. A width dependent characteristic Damkohler number coupled lateral heat and mass transfer has been developed to analyze this transition. The Damkohler number increases as the width increases only if the width is narrow. When the width is higher than a critical value, its effect on the Damkohler number can be neglected. For this reason, the transition pressure first shifts from 25kPa (10 mm and 20 mm width) to 20kPa (30 mm width), and then keeps unchanged at 15kPa (width>50 mm). This work strengthens our understanding on the effect of width on fire risks in aircraft.

- **Keywords:** Sub-atmospheric flame spread; Transition; Heat transfer; Mass transfer; Sample width; Combustion

### Tong Liu, Xing Zheng, Gang Tang, Xinyu Yang, Hegang Zhi, Xiaopeng Qiu, Xiaoliang Li, Zi Wang. *Effects of temperature shocks on the formation and characteristics of soluble microbial products in an aerobic activated sludge system*. Pages 231-241.

The present study investigated the impacts of temperature shocks on the generation of soluble microbial products (SMPs) in an aerobic activated sludge system, focusing on biopolymers and low molecular weight (LMW) substances that significantly impact the effluent quality. The results indicated that raising the temperature increased SMP production. At 25 and 35 °C, all size fractions of SMPs increased linearly with the aeration time, and biopolymers comprised a large proportion of SMPs. At 5 and 15 °C, in contrast, only biopolymers increased linearly with the aeration time, and LMW substances were the predominant fraction of SMPs. The reduced bio-utilization of SMPs with an increase in temperature was associated with the decreased relative abundance of LMW substances, which is supported by the assimilable organic carbon bioassay measurements. The mass of the biopolymers for the SMPs and extracellular polymeric substances (EPS) was balanced at all temperatures, wherein a negative correlation was observed, indicating that increased SMPs in the water phase led to a decrease in EPS. The results of the reactive oxygen species (ROS) and toxicity assays confirmed that the immune defense reaction of the bacteria (induced by ROS) was the key factor for variations in LMW substances in the SMPs and EPS under temperature stresses.

- **Keywords:** Biopolymer; Low molecular weight substances; Soluble microbial products; Extracellular polymeric substances; Reactive oxygen species; Temperature

**Ming-Qing Zhang, Wei Zhang, Min-Sen Chiu, Xiong-Lin Luo. *Scalable active subspace low-rank graph representation for continuous system online security evaluation with input corruption*. Pages 242-256.**

Continuous online system operation evaluation aims to monitor the occurrence of abnormal conditions. However, most of the currently popular monitoring methods are developed from the perspective of historical data integrity. In industrial processes, missing or corrupted entries generally exist due to improper recording or sensor drop-out, which brings difficulties to online monitoring evaluation. In this article, a scalable active subspace low-rank graph representation method is presented to deal with missing data in the offline phase of fault monitoring. The method realizes the reconstruction of a clean matrix by the linear combination of low-rank representation and scalable orthogonal matrix. Meanwhile, the low-rank representation and sparse error matrix with l2,1-norm are arranged in the loss function to improve the optimal feature selection and robustness of the model. Apart from that, to preserve the consistency of the adjacent structure between the reconstruction space and the original corrupted space, a Laplacian manifold regularization is designed to constrain the sparse error. Finally, we establish an optimal graph discriminant model of recovery data for online safety monitoring of continuous systems. Confirmatory simulations on benchmark TE process and actual multi-phase flow process illustrate that the proposed approach is superior to the state-of-the-art methods, fully verifying the robustness and detectability performance in the presence of specific corruption.

- **Keywords:** Online security evaluation; Fault monitoring; Low-rank representation; Laplacian regularized sparse error; Scalable active subspace low-rank graph

**Armin Ebrahimi, Bahram Ghorbani, Masoud Ziabasharhagh. *Exergy and economic analyses of an innovative integrated system for cogeneration of treated biogas and liquid carbon dioxide using absorption–compression refrigeration system and ORC/Kalina power cycles through geothermal energy*. Pages 257-281.**

Nowadays, it is undeniable that applying renewable energy kinds with the approach of maximizing the performance of energy systems owing to the rising trend of energy demand in the world. In this research, an innovative integrated structure for the cogeneration of biomethane (bioCH4) and liquid carbon dioxide (CO2) by unrefined biogas and exhaust fumes from power plants is developed. The cryogenic biogas upgrading process and CO2 capture cycle are used for the treatment of unrefined biogas and the exhaust fumes from the power plants, respectively. The absorption–compression cooling process and organic Rankine/Kalina power units through geothermal energy are used to provide refrigerate and power. The present integrated process generates 0.8434 kg/s bioCH4 and 2.631 kg/s liquid CO2 by receiving 2.368 kg/s untreated biogas, 21.32 kg/s flue gas, and 7922 kW heat flow from geothermal energy. The thermal and total exergy efficiencies of the hybrid system are achieved at 59.94% and 73.10%, respectively. Exergy analysis depicts that the heat exchangers (4043 kW) and distillation columns (1857 kW) have the most exergy destruction in the among of equipment, which is 39.12% of the total system destruction. The heat exchanger network related to the multi-stream exchanger HE16 is extracted by pinch method. The economic assessment illustrates that the return period and the prime cost of the product are equal to 4.45 years and 0.8189 US$/ m3 bio-methane, respectively. The sensitivity investigation illustrates that the total thermal efficiency increases up to 72.50% and geothermal heat duty decreases to 7808 kW with the increase of methane composition in the untreated biogas from 55 mol% to 75 mol%. The return period increases up to 2.235 years and the net annual benefit decrease to 16.73 MMUS$/year when the bio-methane cost decreases from 2.5 US$/m3 to 0.5 US$/m3.

- **Keywords:** Biogas upgrading process; Absorption–compression refrigeration system; Kalina/ORC power cycles; Geothermal energy; Exergy and economic analyses

**Jiangsheng Li, Quanquan Wu, Yueyan Huang, Zewen Sun, Jianlong Li, Daishe Wu. *Particulate matters filtration by a filter medium with pin holes: modeling and experimental verification*. Pages 282-290.**

Air filtration systems have difficulty avoiding problems of leakage and breakage of the filter medium, which aggravates the emission of dust particles. In this study, a numerical calculation model is established to study the dust-laden air filtration performance of a filter medium with pin holes. The calculation model is verified using experiments and by comparing the values of the filtration resistance and efficiency. The results demonstrated that, with the existence of leakage, the filtration efficiency decreased with time, decreased with an increase in the leakage ratio, and increased first and then decreased with an improvement in the filter medium accuracy. An extremely high filter medium accuracy was not conducive to improve the filtration efficiency, but it obviously increased the filtration resistance. The larger the leakage ratio, Lr, the smaller the optimal filter accuracy, eF,opt, and the maximum filtration efficiency, eT,max. The functional relationships between eF,opt, eT,max and Lr, as well as QT, were obtained. With an increase in the leakage ratio, the filtration resistance and its rising rate decreased. The system quality factor decreased with the increase of the leakage ratio and increased with the increase of the filter quality factor.

- **Keywords:** Particle filtration; Filter medium leakage; Numerical calculation; Airflow resistance; Filtration efficiency

**D.B. Sivakumar, M. Arulmozhi, S. Sathyanarayanan, M. Sridharan. *Optimization of gasoline engine operating parameters fueled with DIPE-gasoline blend: Comparative evaluation between response surface methodology and fuzzy logic expert system*. Pages 291-307.**

Engine performance and emission characteristics of diisopropyl ether (DIPE)–gasoline blends were evaluated for several loads using a single-cylinder, four-stroke, multi-fuel variable compression ratio engine. The engine was operated with five test fuels: DIPE0 (neat gasoline), DIPE10 (90% gasoline + 10% DIPE), DIPE15 (85% gasoline + 15% DIPE), DIPE20 (80% gasoline + 20% DIPE), and DIPE25 (75% gasoline + 25% DIPE) by volume. The responses such as brake thermal efficiency (BTE), specific fuel consumption (SFC), carbon monoxide (CO), hydrocarbons (HC), and oxides of nitrogen (NOx) were optimized using response surface methodology (RSM) and fuzzy logic expert system (FLES) considering compression ratio (CR), brake power (BP), and DIPE blend percentage as input variables. The developed RSM model provided a significant fit with higher R2 (correlation coefficient) values. The RSM models showed better performance than the FLES model. The optimized responses such as BTE, SFC, CO, HC, and NOx were 26.9%, 0.378 kg/kW h, 0.0135% by volume, 152.66 ppm, and 3465 ppm, respectively. The optimized results were validated with the experimental results, and the error percentage for all the responses were low. Thus, the developed RSM models gave better results than FLES and can predict and optimize engine performance and emission characteristics.

- **Keywords:** Response surface methodology; Fuzzy logic expert system; Alternate fuel; gasoline blend; gasoline engine; emission control

**Yue Zhang, Huilan Li, Yankui Tang, Penghong Luo, Weiwei Yang, Yu Wu, Fan Yang, Jianhua Xiong. *Aeromonas hydrophila-derived BioMnOx activates peroxymonosulfate for 2,4-dimethylaniline degradation in water: mechanisms and catalyst reusability*. Pages 308-319.**

Biogenic manganese oxide (BioMnOx) has been identified as an ideal material for pollution elimination and environmental remediation, due to its remarkable reactivity and structural diversity. In this study, a Mn(II)-oxidizing bacterium-Aeromonas hydrophila DS02-derived BioMnOx was used to serve as a heterogeneous catalyst for peroxymonosulfate (PMS) activation to degrade a refractory organic pollutant, 2,4-dimethylaniline (2,4-DMA), in the aqueous solution. The results showed that more than 98% of 2,4-DMA can be degraded in 120 min over a pH range of 5–9. Analysis of FTIR, SEM, XPS and XRD revealed that the morphologies and chemical structures of the BioMnOx materials changed during the reaction and recycle process, but the catalytic effectiveness and stability were maintained over three cycles in the PMS/BioMnOx system at initial pH 5. Free radicals, $SO_4^{\cdot-}$ and ·OH, were both involved in the 2,4-DMA degradation, with $SO_4^{\cdot-}$ playing the dominant role. The proposed degradation pathways revealed that 2,4-DMA could be decomposed to the more biodegradable benzoic acid. The studied BioMnOx/PMS system is environment-friendly and it shortens the treatment time compared with the previously reported methods and improves the biodegradability of 2,4-DMA.


- **Keywords:** Aeromonas hydrophila; Biogenic manganese oxide; Heterogeneous catalyst; Peroxymonosulfate (PMS) activation; 2,4-dimethylaniline (2,4-DMA)


### Liu Jing, Jun Zhao, Heyang Wang, Wenjia Li, Yanping Du, Qiang Zhu, Mohamed E. Zayed. *Numerical analysis of the effect of swirl angle and fuel equivalence ratio on the methanol combustion characteristics in a swirl burner*. Pages 320-330.

The outstanding advantages of methanol such as low pollutant emissions of nitrogen oxides (NOx) and carbon monoxide (CO) make it a promising clean-burning fuel. Despite, the latent heat of vaporization of methanol is 3.70 times that of gasoline, the low heating value of methanol is one of the most critical barriers to its effective utilization in industrial applications. Thus, the methanol burner needs to be effectively designed to determine the desired combustion characteristics and the optimal design of this type of clean burner. Hence, this study presents a computational fluid dynamic analysis on the combustion characteristics of a methanol swirling burner with two layers of swirling blades. A particular focus of this study is emphasized on the effects of different swirling blade angles (45°+45°, 60°+60°, and 45°+60°) and various equivalence ratios (0.5, 0.75, 1.0, 1.25, and 1.75) on the combustion characteristics and pollutants formation of the swirl burner. The velocity and temperature profiles, combustion characteristics, and concentrations of major combustion species are analyzed in detail. The results show that the blade angle arrangement of 45°+ 60° exhibits the best combustion characteristics in comparison with the other blade angle arrangements. It is also found that the BA3 with an equivalent ratio in the range of 1.0–1.25 shows the best performance in the emissions of NOx and CO compared with other combinations of swirling blade arrangements and equivalence ratios. More specifically, the optimal equivalence ratio ranges from 1.0 to 1.25 at which the NOx and CO emissions are measured to be 27.0 and 11.0 mg/m3, respectively.


- **Keywords:** Methanol combustion; Swirling burner; Blade swirl angle; Fuel equivalent ratio; Computational fluid dynamic


### Qiao Wang, Xinjiao Luo, Changjian Wang, Yi Liu, Penggan Zhou, Bing Li. *Experimental study on external explosion for vented hydrogen deflagration in a rectangular tube with different vent coefficients*. Pages 331-339.

Experiments on hydrogen-air vented deflagration in a smooth rectangular tube were conducted with various vent area for different hydrogen concentration. The high-speed

schlieren camera was employed to visualize the external flow field. The internal and external overpressures were obtained from five pressure transducers. The effects of vent area for different hydrogen concentration were discussed on the build-up of internal/external overpressures and the evolution of external flow field. Two types of internal overpressure structure, affected by Helmholtz oscillation and external flow field, were observed for different vent coefficient and hydrogen concentration. The increase of hydrogen concentration promotes external mixture reactivity and the external overpressure. The increase of vent coefficient drives the increase of outlet speed of vented gas and flame and generally promotes external overpressure. The higher speed flame provides stronger ignition energy to external combustible gas cloud. For the high hydrogen concentration of 18 vol%, external overpressure increases linearly with vent coefficient. The rise of external overpressure can cause the increase of internal overpressure when it is large enough, particularly in the case of large vent coefficient, and the internal overpressure peak affected by external explosion can even dominate the maximum internal overpressure.

- **Keywords:** Hydrogen safety; Vented deflagration; Vent coefficient; External overpressure; Hydrogen concentration

### Jun Yang, You Xue, Xinyu Dai, Hongxing Lu, Ming Yang. *An intelligent operational supervision system for operability and reliability analysis of operators manual actions in task implementation*. Pages 340-359.

In the paper, we present a framework for comprehensive operational feasibility analysis from both functional and structural safety perspectives using the measures of hazard and reliability. Within the framework, a pattern-matching algorithm is proposed for operation supervision and underlying human error mode identification using procedure-based action library. An intelligent operational supervision system is further developed in integration with operational mission reliability analysis. The capabilities of procedure-guided operation navigation and supervision as well as operability and reliability of operators manual actions are validated by a case study of reactor boron and water makeup system for manual makeup task implementation in QT virtual simulation environment. The validation results show that the intelligent operational supervision system is capable of procedural operation navigation and supervision. The trend impact of proactive operations can be effectively profiled using the measures of reliability in synchronous prediction and supervision.

- **Keywords:** Human error mode; Emergency response planning; Functional hazard analysis; Mission reliability analysis; GO-FLOW; Multilevel flow models

### Dalin Li, Wei Chen. *Effects of impeller types on gas-liquid mixing and oxygen mass transfer in aerated stirred reactors*. Pages 360-373.

Aeration and stir are vital steps in wastewater treatment plants (WWTPs) to enhance dissolved oxygen (DO) concentration in water. In laboratories, aerated stirred reactors (ASRs) are commonly utilized to cultivate activated sludge and degrade pollutants in sewage. The performance of the ASR depends mainly on the gas-liquid distribution and hydrodynamics. The current study investigated a lab-scale ASR using computational fluid dynamics (CFD) modeling and simulation. The experimental data were used to validate the CFD model. Then, the validated model was used to investigate the effect of impeller types on gas-liquid mixing quality and oxygen mass transfer efficiency. This investigation aimed to select suitable and efficient impeller types for different needs in ASRs. The predictions suggested the Pitched 30° impeller is excellent in mass transfer and gas-liquid mixing besides needing more power. Simulation results of oxygen transfer shown that the gas holdup and bubble diameter mainly determined the oxygen mass transfer coefficient in ASRs. Rushton impeller and Folded impeller offer good oxygen transfer but

also higher power consumption. Pitched 45° impeller and Pitched 60° impeller offer more uniform gas holdup than other impellers and have lower energy consumption.


- **Keywords:** Aerated stirred tank; CFD model; Mixing; Oxygen mass transfer; Impeller type


### Huanhuan Chen, Liping Chen, Wenqian Wu, Zichao Guo, Xiaoqiao Zhao, Wanghua Chen. *Adiabatic kinetics calculations considering pressure data*. Pages 374-381.


Pressure and temperature play an important role in the adiabatic decomposition of hazardous materials. In this article, Accelerating Rate Calorimeter (ARC) was used to study adiabatic decomposition of 40 wt% dicumyl peroxide (DCP) solution , 20 wt% di-tert-butyl peroxide (DTBP) solution and 2,4-dinitrotoluene (2,4-DNT). Based on the temperature and pressure signals, the kinetic constants of 40 wt% DCP and20 wt% DTBP were calculated separately. It is found that the temperature and gas production kinetics of the 40 wt% DCP solution are in good agreement with each other, but the temperature and gas production kinetics of 20 wt% DTBP solution are significantly different. The adiabatic decomposition of 2,4-DNT under different pressure conditions was experimentally investigated. The experimental results indicated that pressure promoted the adiabatic decomposition of 2,4-DNT. Accordingly, new kinetic equations were developed to describe the adiabatic decomposition of 2,4-DNT under different pressure conditions. These works provide a new insight into adiabatic kinetics calculations.



- **Keywords:** Adiabatic calorimetry; Pressure effects; Decomposition mechanism model; Kinetic parameters


### July Bias Macêdo, Márcio das Chagas Moura, Diego Aichele, Isis Didier Lins. *Identification of risk features using text mining and BERT-based models: Application to an oil refinery*. Pages 382-399.


The uncontrollable release of hazardous substances may lead to catastrophic accidents. In this context, risk studies are aimed at recommending either preventive measures or designing safeguards to mitigate the consequences. To that end, risk experts postulate possible leakages, then identify their causes and consequences, and finally evaluate and classify the risks into categories. These analyses rely on examination different engineering textual documents and attendance numerous meetings, which is very time consuming. Moreover, this qualitative process of hazard identification and assessment are usually the first steps of quantitative risk analysis (QRA) and is paramount to ensure its quality. Therefore, we here propose to use text mining and fine-tuned trained bidirectional encoder representations from transformers (BERT) models to support and reduce the efforts required for completing the early stages of QRA. Our idea is to apply these techniques to identify the potential consequences of accidents related to the operation of an oil refinery and classify each scenario in terms of severity of the consequence and likelihood of occurrence. The proposed method was applied to an actual oil refinery and presented very promising results. The potential consequences, the severity and likelihood categories were predicted with a mean accuracy of 97.42%, 86.44%, and 94.34% respectively. The models resulting from this research were embedded into a web-based app that is called HALO (hazard analysis based on language processing for oil refineries).



- **Keywords:** Hazard identification; Hazard assessment; Natural language processing; Text mining; Oil refineries


### Abdellah-Anouar El Foulani, Jamal Jamal-eddine, Brahim Lekhlif. *Study of aluminium speciation in the coagulant composite of polyaluminium*

***chloride-chitosan for the optimization of drinking water treatment*. Pages 400-408.**

The control of aluminium speciation in coagulant composites is the appropriate approach to remove turbidity and natural organic matter from raw water effectively. This suspended matter in water affects its organoleptic quality and triggers problems by causing interference with the water treatment process. This study examined the behaviour of composite coagulants polyaluminium chloride-chitosan (PAC-CTS) with different aluminium speciation and polymer ratio to remove oxidizable matter and turbidity residing in surface waters. The fraction of basicity ratio (Al/OH) in the preparation of polyaluminium chloride (PAC) and chitosan (CTS) were simultaneously evaluated and optimized according to aluminium speciation by experimental design. The interaction between PAC and CTS was examined via Al-Ferron timed spectrophotometric approach, theoretical study and fourier transform infrared (FTIR) analysis. Ferron analyses reveal that basicity ratio and CTS fraction affect the distribution of aluminium forms (mononuclear Ala, medium polymeric Alb, colloidal, and high polymeric Alc) in PAC-CTS. The theoretical study showed that Al(OH)2+, Al13, and Al30 species are more reactive than aluminium hydroxide Al(OH)3 at different magnitudes and sites with chitosan. The FTIR analysis confirmed the existence of an interaction between PAC and CTS by revealing a new peak for Al-NH2 stretches. The coagulation performance study of composite coagulant PAC-CTS with different compositions showed that the increase of chitosan and the preponderance of Alb and Alc species compared to Ala are suitable for removing colloidal suspensions. Further, incorporation of PAC with high basicity (74.1%) in 16.3% of chitosan (PAC-CTS1) removed 99.51% of turbidity and 66.66% of oxidizable matter at AlCl3 concentration of 10 mg l−1. However, increasing the percentage of chitosan to 34.1% at the same basicity (74.1%) in the PAC-CTS4 compound was not beneficial for oxidizable matter removal. It was speculated that the improvement in coagulation performance could be achieved by considering the aluminum speciation and polymer content in the composite flocculant PAC-CTS. The present work could be a useful model for synthesizing and studying organometallic interactions in developing new composite coagulants to improve coagulation performance.

- **Keywords:** Composite coagulant; Polyaluminium chloride (PAC); Chitosan (CTS); Basicity; Ferron method; Colloidal suspension removal

**Rongwei Bu, Chuangang Fan, Zhengwei Guo, Yang Zhou. *Energy distribution analysis on suppressing a shielded fire with water mist in a tunnel rescue station*. Pages 409-417.**

In real tunnel fire scenarios, water mist has little opportunities to directly apply to train fires shielded by a carriage body. However, most models for heat transfer analysis assume direct contact between fire source and mist droplets. It is of interest to find a method to evaluate the energy exchange between water mist and a shielded fire. To investigate the water mist suppression performance on a shielded fire, a full-scale experimental and theoretical study was performed by varying the activation time of water mist system, working pressure, and the diameter of mist droplets. The suppression performance is found to be dependent on the working pressure for the small mist droplets, and sensitive to the size of mist droplets at high working pressure. Moreover, the suppression performance is also influenced by the water mist activation time due to the competition of fuel cooling and the inhibition effect of the smoke layer. A theoretical model was developed to predict the energy exchange among smoke, water mist, and surroundings. It was found that in comparison to the indirectly restricted effect of cooling the carriage and fire, the direct heat loss between water mist and smoke is the main controlling mechanism. This study provides an important reference for the design of fire water system in the tunnel rescue station and is beneficial to the environmental protection of fire extinguishing sites.

- **Keywords:** Water mist; Working pressure; Rescue station; Energy distribution; Heat loss

**Jianfeng Yang, Ru Li, Liangchao Chen, Yuanhao Hu, Zhan Dou. *Research on equipment corrosion diagnosis method and prediction model driven by data*. Pages 418-431.**

With the rapid development of the oil refining industry, safety problems caused by equipment corrosion have become increasingly important, making equipment corrosion management a key factor to ensure process safety. Corrosion diagnosis, as the first step of equipment corrosion management, is of great significance in not only ensuring the proper corrosion supervision, but also realizing safety protection of equipment. This paper addresses the problems of incompleteness as well as the subjective factors of existing methods in equipment corrosion diagnosis. The proposed solution, based on data-driven corrosion diagnosis, suggests a more comprehensive view. Special focus in this paper is on evaluation and prediction of corrosion safety state, including the identification of corrosion mode and the prediction of corrosion type and degree. This paper brings together large amount of historical data of equipment corrosion detection and solves the problem of unbalanced original data by data wrangling and the application of Borderline-SMOTE algorithm. What's more, a prediction model that is based on Random Forest (RF) algorithm is constructed, aiming at equipment corrosion mechanism, type and degree. The results show that the model, aiming at critical mechanism identification, performs ideally after evaluation and the accuracy of the results amount to 86%. As for the classification and prediction of corrosion state, the model can be further optimized by Particle Swarm Optimization (PSO) algorithm to reach a better accuracy (92%), which verifies generalization effect compared with traditional prediction models. In addition, this solution improves the functionality and practicability of corrosion diagnosis, which is beneficial to the investigation of hidden dangers. It also can serve as an instruction for equipment safety management to ensure the stable operation for an enterprise.

- **Keywords:** Corrosion diagnosis; Data-driven; Unbalanced data processing; Random Forest

**V. Bisio, F. Montomoli, S. Rossin, M. Ruggiero, V.L. Tagarielli. *Predictions and uncertainty quantification of the loading induced by deflagration events on surrounding structures.* Pages 445-460.**

The threat of accidental hydrocarbon explosions is of major concern to industrial operations; in particular, there is a need for design tools to assess and quantify the effects of potential deflagration events. Here we present a design methodology based on analytical models that allow assessing the loading and structural response of objects exposed to pressure waves generated by deflagration events. The models allow determining: i) the importance of Fluid-Structure Interaction (FSI) effects; ii) the transient pressure histories on box-like or circular cylindrical objects, including the effects of pressure clearing; iii) the dynamic response of structural components that can be idealised as fully clamped beams. We illustrate by three case studies the complete design methodology and validate the analytical models by comparing their predictions to those of detailed CFD and FE simulations. We employ the validated analytical models to perform Monte Carlo analyses to quantify, for box-like structures, how the uncertainty in input design variables propagates through to the expected maximum force and impulse. We present this information in the form of non-dimensional uncertainty maps.

- **Keywords:** Hydrocarbon; Pressure waves; Deflagration; Uncertainty quantification; Process safety

**Song Ding, Xing Pan, Dujun Zuo, Wenjin Zhang, Liuwang Sun. *Uncertainty analysis of accident causality model using Credal Network with IDM method: A case study of hazardous material road transportation accidents*. Pages 461-473.**

Bayesian network (BN) is an effective tool for causal inferences of accidents. However, it is often criticized for the difficulty in obtaining accurate/sufficient data needed to get precise probability numbers, and expert knowledge is necessary on this occasion. Such numbers provided by experts lead to great cognitive uncertainty in the model. Credal Network (CN), regarded as an extension of BN, uses imprecise probabilities to well express the cognitive uncertainty, but how to give the available interval probability is a key issue in its application. In this paper, a CN model based on Imprecise Dirichlet Model (IDM) is proposed to solve this problem, and a case study of hazardous material road transportation accidents (HMRTAs) is conducted. Firstly, based on the accident causation model, the CN topology is established by analyzing 30 investigation reports of HMRTAs in China. Secondly, the conditional probability table is calculated and then the CN model of HMRTAs is obtained by transforming the point probability into interval probability using IDM. Finally, causes and consequences of HMTRAs are analyzed. The results show that the method in this study can well represent the uncertainty propagation in the accident causal model and provide a new way for accident risk analysis.

- **Keywords:** Hazardous material; Credal Network; Interval probability; Uncertainty; Causal model

**Moogambigai Sugumar, Vaidhegi Kugarajah, Sangeetha Dharmalingam. *Optimization of operational factors using statistical design and analysis of nanofiller incorporated polymer electrolyte membrane towards performance enhancement of microbial fuel cell*. Pages 474-485.**

Response Surface Methodology (RSM) coupled with Box–Behnken (BB) design is adopted to optimize Microbial Fuel Cell (MFC) performance statistically as a function of three selected operational factors such as filler concentration, membrane thickness and anode surface area. Various concentrations (2%, 4%, 6% and 8%) of Sulphonated Zinc Oxide Nano Rods (SZnO NR) with Sulphonated Polystyrene Ethylene Butylene Polystyrene (SPSEBS) are used as Proton Exchange Membranes (PEM) in a fabricated tubular MFC with a holding volume of 300 mL. The prepared nanocomposite membranes are analyzed for their water uptake, ion exchange capacity (IEC), oxygen crossover and proton conductivity to confirm the membrane suitability for MFC operation. The results indicate that SPSEBS + 6% SZnO NR possesses highest proton conductivity of 1.49 × 10-2 S/cm compared to other nanocomposite membranes and is thus selected for statistical analysis. Statistical analysis shows that STAT 15 with filler concentration of 6.5%, membrane thickness of 120 μm and anode surface area of 19.7 cm2 exhibits the highest maximum power density of 147 mW/m2. The results suggest a novel nanocomposite membrane that could be a suitable PEM and also gives a regression equation for optimizing factors which enhances electricity generation in MFC.

- **Keywords:** Response Surface Methodology (RSM); Cation Exchange Membrane (CEM); Operational factors; Microbial Fuel Cell (MFC); Physicochemical analysis; Biofilm analysis

**Carmen Hernández-Crespo, Núria Oliver, María Peña, Miguel Añó, Miguel Martín. *Valorisation of drinking water treatment sludge as substrate in subsurface flow constructed wetlands for upgrading treated wastewater*. Pages 486-494.**

Drinking water treatment sludge (DWTS) is the main waste produced in drinking water treatment plants (DWTPs). Its valorisation as substrate for constructed wetlands (CWs) aimed at upgrading treated urban wastewater is presented. Keeping a holistic approach in mind, this study looks for nutrient and organic matter removal but also contaminants of emerging concern (CECs) and pathogens. Three pilot subsurface flow CWs (1 m2) were installed under outdoor conditions in real WWTPs. Different operation modes (sequential: S-CW and continuous saturated flow: C-CW, CC-CW), different nutrient influent concentrations (S-CW and C-CW: 0.6 mg TP/l, 12.7 mg TN/l; CC-CW: 6.5 mg TP/l, 48 mg TN/l) and high hydraulic loading rates (HLRs, 0.9–5.1 m3/m2/d) were tested. C-CW presented higher removal efficiencies than S-CW for TP (C-CW: 56–86%; S-CW: 32–66%), total nitrogen (C-CW: 23–38%; S-CW: −3 to 6%) and E. coli (C-CW: 94%; S-CW: 84%), while S-CW performed better for ammonium (C-CW: 29–45%; S-CW: 72–86%) and CECs removal. Among fifteen CECs monitored, most pharmaceuticals, four were significantly reduced in C-CW and nine in S-CW, which had more aerobic conditions. CC-CW reduced nutrients and organic matter by 62% (TP), 8% (TN), 23% and 40% (chemical and biochemical oxygen demands, respectively). The potential release of aluminium was negligible. Novel values for the first-order reaction coefficient of P-k-C* model are provided for the TP removal process using DWTS (0.6–1.0 h−1). The main conclusion is that DWTS is a suitable substrate to significantly upgrade WWTP effluents, even at high HLRs. A hybrid system combining sequential and continuous flow modes could optimize the upgrading treatment. A proposal for the full valorisation of the sludge produced in one DWTP is presented.


- **Keywords:** Alum sludge; Treatment wetlands; Emerging pollutants; Upgrading treatment; Phosphorus removal; Pathogens removal


**Yanling Zhao, Guangchao Jia, Yili Shang, Peitao Zhao, Xin Cui, Qingjie Guo. *Chlorine migration during hydrothermal carbonization of recycled paper wastes and fuel performance of hydrochar*. Pages 495-502.**

Wastes from recycled paper industry (WRP) was hydrothermally carbonized to remove impurities to produce alternative biofuel. The chlorine behaviors during hydrothermal carbonization (HTC) and the fuel properties of the generated hydrochar were evaluated. The degradation of lignocellulosic components improved free -OH bond and small free cellulosic fragments facilitating dechlorination. Meanwhile, dechlorination process stimulated degradation of biomass. The carbon content and density of WRP were improved by HTC resulting in high heating value increasing from 5044.40 MJ/m3 to 17,004.88 MJ/m3. Pollutants emission from hydrochar combustion would be effectively controlled because of the removal of sulfur and chlorine. Hydrochar enjoyed higher ignition temperature and average combustion rate while lower burnout temperature, indicating that the combustion range has been narrowed, thus improving the combustion efficiency. The increase of HTC temperature facilitated hydrochars combustion and reduce energy consumption during hydrochar combustion. Mild HTC operating conditions (220 ℃ for 90 min and 240 ℃ for 60 min) were supposed to effectively improve the combustion intensity with stability meanwhile reached the highest dechlorination efficiency. These results evidence the feasibility of converting WRP to clean biofuel via HTC.


- **Keywords:** Recycled paper wastes; Hydrothermal carbonization (HTC); Chlorine migration; Hydrochar fuel properties


**Jianqi Chen, Wei Yuan, Hongpeng Ma, Bing Liu, Zhihong Dang, Aosong Wei, Bin Hu, Shihao Ma, Hualin Wang, Wenjie Lv. *Industrial application of swirl regenerating micro-channel separation (SRMS) for fine catalysts removal from methanol-to-olefin quench water*. Pages 503-514.**

Methanol to olefin (MTO) process is a chemical technology for producing low-carbon olefins from coal-based or natural gas-based methanol, which has changed the pattern of low-carbon olefins relying on petroleum cracking. However, a large amount of fine catalyst powders circulating in the water system of the MTO plant threats the sustainability of the process severely. Previously, a pilot-scale study about swirl regenerating micro-channel separation (SRMS) technology to remove the fine waste catalyst powders from MTO quench water was reported. In this study, the SRMS equipment was scaled up to an industrial level with a processing capacity of 400 m3/h based on the results of pilot-scale experiments, and the performance of the industrial unit was monitored for over 6 months. The results obtained directly from the industrial site showed that the SRMS unit based on deep-bed filtration and swirling flow enhanced washing and desorption could effectively remove the fine catalyst particles in the quench water, and the effluent particle concentration was maintained below 20 mg/L. Furthermore, the total oil content in the quench water reduced from 43.2 mg/L to 22.8 mg/L after being processed by the SRMS unit, which demonstrates that the SRMS unit also has an appreciable ability for oil pollutants removal. After the long-term operation of the SRMS unit, the equilibrium concentration of particulate matter in the quench water was reduced to under 50 mg/L, which significantly improved the performance of the quench water heat exchanger and effectively reduced the cleaning frequency of the heat exchanger, air cooler, and other equipment in the water system. Through the industrial-scale technical comparison, this technology outperforms the other common quench water treatment methods in equipment investment, maintaining cost, freshwater supplement, and energy consumption.


- **Keywords:** Swirl regenerating micro-channel separation; Deep-bed filtration; Methanol-to-olefin; Quench water; Fine catalyst powders


**Yongkui Yang, Kyong-Ryong Kim, Rongrong Kou, Yipei Li, Jun Fu, Lin Zhao, Hongbo Liu. *Prediction of effluent quality in a wastewater treatment plant by dynamic neural network modeling*. Pages 515-524.**


Improving the operation, management, and consequent performance of wastewater treatment plants (WWTPs) for conserving the water environment is crucial. Recent advancements in artificial intelligence (AI) modeling have shown the potential to solve the non-linear simulation of processes in WWTPs and facilitate real-time operational adjustments. In this study, a dynamic nonlinear autoregressive network with an exogenous input (NARX) model was established for predicting effluent quality. The performance was optimized with different time-delay parameters and training algorithms. Then, a PCA-NARX hybrid model was established for high performance and comparison with two static artificial neural network (ANN) models. The BR algorithm exhibited the highest performance among the four training algorithms for the NARX model. The dynamic PCA-NARX model was significantly superior to static models in modeling effluent quality. The PCA-NARX model predicted the effluent chemical oxygen demand (CODcr) and total nitrogen (TN) with high accuracy (RMSECOD = 2.9 mg/L, RMSETN = 0.8 mg/L). Therefore, we propose a stable and sensitive dynamic neural network model for predicting effluent quality and potential real-time adjustment of wastewater treatment operations.



- **Keywords:** Wastewater treatment plant; Artificial neural network; Nonlinear autoregressive network with an exogenous input; Artificial intelligence; Principal component analysis


**Xueli Geng, Hao Zhou, Peng Yan, Hong Li, Xingang Li, Xin Gao. *Exergy, economic and environmental analysis of an integrated pressure-swing reactive distillation process for the isobutyl acetate production via methyl acetate transesterification*. Pages 525-536.**

As a greener bio-based solvent, isobutyl acetate (ISBAC) was widely applied in biorefineries around value-added production for environmental protection and ecological safety. The convention production of ISBAC, which was obtained by the reaction of alcohols and acids, can form by-product water to cause the multiple heterogeneous azeotropes and further enormously increase separation difficulty and production costs. This work adopted the transesterification of methyl acetate (MeAC) from the by-product (typical compositions MM20 (15.64 mol% MeAc, 84.36 mol% MeOH) and MM80 (65 mol% MeAC, 35 mol% MeOH) of polyvinyl alcohol (PVA) manufacture and isobutanol (ISBOH) to product ISBAC to avoid the multiple heterogeneous azeotropes. The ISBAC production by MeAC in MM20 and MM80 reacted with ISBOH adopted reactive distillation (RD) combining pressure-swing to break the limits of chemical equilibrium and azeotrope separation. Furthermore, heat integration, thermal coupling, and heat pump technologies were used to systematically recover waste heat and achieve energy-saving for ISBAC production processes. The exergy, economy, and environment evaluation displayed that the heat integration of MM20 pressure-swing RD was the best attractive process by reducing 19.35% total annual cost (TAC), 34.58% CO2 emissions, and improving 33.16% thermodynamic efficiency. The heat source of the low-pressure column and preheating process feed using top steam of the high-pressure column ( heat integration-F ) of MM80 pressure-swing RD process was the most promising process due to the decrease of 5.40% in TAC, 16.70% in CO2 emissions and obtained the improvement of 4.50% thermodynamic efficiency comparing with the conventional process.


- **Keywords:** Transesterification; Reactive distillation; Process intensification; Isobutyl acetate; Pressure-swing process


### Piotr Machniewski, Eugeniusz Molga. *CFD analysis of large-scale hydrogen detonation and blast wave overpressure in partially confined spaces*. Pages 537-546.

The effect of confinement on the magnitude of overpressure due to a gaseous detonation of a hydrogen-air mixture was studied with the aid of numerical simulations. A simplified combustion reaction kinetic model applied along with computational fluid dynamics (CFD) allowed for the numerical simulation of large-scale detonations of hydrogen-air mixtures. The model was validated against experimental data reported in the literature for the case of a large-scale (300 m3) surface (unconfined space) detonation of a hydrogen-air mixture and the results of a hydrogen-air (confined space) detonation test performed in a 263 m3 tunnel facility. The predicted overpressure and detonation velocity was in agreement with the measurements in both unconfined and confined detonation cases. To verify the effect of confinement on the magnitude of the blast wave overpressure due to detonation of a combustible gas cloud, a series of CFD simulations of hydrogen detonations followed by propagation of a non-reactive blast wave in various geometries were carried out. The results were compared with the correlation applicable for unconfined detonations, which was also found to be applicable for partially confined detonations after the transformation of the distance from explosion centre to spherical blast wave equivalent radius.


- **Keywords:** Accident scenario; CFD; Detonation; Hydrogen safety


### A.B. Mpofu, W.M. Kaira, O.O. Oyekola, P.J. Welz. *Anaerobic co-digestion of tannery effluents: Process optimisation for resource recovery, recycling and reuse in a circular bioeconomy*. Pages 547-559.

The anaerobic treatment of tannery effluents from the different process stages are limited by the various toxicants that are mainly added as feed chemicals. The segregated effluents present an opportunity for co-treatment to abate inhibition, supplement deficient nutrients and/or promote resource recovery using anaerobic digestion. This

study investigated the feasibility of anaerobic co-digestion of beamhouse (BH) and pre-treated tanyard (TY) effluents using the standardised biochemical methane potential (BMP) protocol. It was established that all reactors were active, while those with higher TY compositions and operating at very high/low inoculum to substrate ratios ($3<ISR \leq 2$) suffered severe methanogenesis inhibition. Process efficiency and kinetics (maximum CH4 production rate and reaction rate constant) improved with increasing BH composition and/or ISR. The logistic, modified Gompertz and cone model showed a better fit to the experimental cumulative CH4data ($0.827 \leq$ Adj R2 $\leq 0.999$), respectively. The optimal operating conditions ($ISR = 2.5$, 100% BH and 20 days retention time) demonstrated the feasibility of a circular bioeconomy and net positive tannery operations where 639 mL biogas/gVS (59% CH4), 13% and 18% of the inlet sulphur and nitrogen, respectively, are recoverable as products. The process also recovered reusable process/irrigation water, recyclable digestate as a biofertiliser and/or ceramic aggregate with energy recovery.


- **Keywords:** Tannery effluents; Anaerobic co-digestion; Kinetics; Optimisation; Resource recovery; Circular bioeconomy


**Xia Zhang, Luwei Peng, Bingqing Xu, Peixuan Liu, Xueran Jiao, Haiyan Kang, Zhongxian Song, Xu Yan, Yanli Mao, Jinli Qiao. *Bi-Cu bimetallic electrocatalysts prepared using electrochemical deposition effluent for highly converting CO2 to formate*. Pages 560-566.**


Developing bimetallic electrocatalysts with synergistic effect is a promising strategy to facilitate the electrocatalytic reduction of CO2 (ECR-CO2). Electrodeposition strategy due to its convenience and time-saving property has been widely used in ECR-CO2, however, the disadvantage of electrodeposition method is the treatment of electroplating liquid waste. Aiming for recovering metal ions from electroplating liquid waste and developing high-performance catalysts for ECR-CO2, a bimetallic Bi3Cu1 is synthesized by green-cleaning method. The Bi3Cu1 catalyst exhibits a promising formate (HCOO-) faradaic efficiency (FE) of 95.1% at −0.75 V vs. RHE in an H-type cell. Moreover, excellent durability is also obtained, maintaining a high FEHCOO- of 89.4% after 20 h electrolysis. In addition, the experimental results show that the KOH is a better choice than the KHCO3 electrolyte for ECR-CO2. Bi3Cu1 shows enhanced current density and FE of formate, owing to the faster mass transport in the gas-fed continuous-flow cell and the high ionic conductivity of KOH electrolyte.



- **Keywords:** Carbon dioxide; Electrochemical reduction; Bi-Cu bimetallic; Electrochemical deposition effluent


**Siti Nur Hatika Abu Bakar, Hassimi Abu Hasan, Abdul Wahab Mohammad, Siti Rozaimah Sheikh Abdullah, Mohd Hafizuddin Muhamad. *Interactions between operating parameters of moving bed biofilm reactors in treating palm oil mill effluent*. Pages 567-575.**


The interaction among operating parameters of moving bed biofilm reactors (MBBR) in a treating palm oil mill effluent (POME) was carried out in order to determine the maximum chemical oxygen demand (COD) and ammoniacal-nitrogen (NH3-N) removal. To achieve these goals, a face-centred central composite design was applied to the hydraulic retention time (HRT: 24–72 h), media filling fraction (MFF: 25–70%), and biofilm carriers (Black plastic media; BPM and Hexafilter; HEX). From the evaluation, the interaction of these operating parameters significantly influenced the removal of COD and NH3-N in the POME. The optimal operating parameters were determined to be 70 h HRT and 29% MFF, while the best biofilm carrier was Hexafilter (HEX). Optimal conditions for COD and NH3-N removal were up to 53.3% (758.4 ± 2 mg L−1) and 91.8% (9.7 ± 2 mg L−1), respectively. The results from this study should provide a template for a viable

alternative to the current, inefficient conventional POME treatment with optimal conditions of the MBBR for the removal of COD and NH3-N.


- **Keywords:** Wastewater treatment optimisation; Zero discharge; Palm oil mill effluent; Biofilm carrier; Water recovery


**Christophe Gueibe, Jos Rutten, Johan Camps, Dominique Moyaux, Wouter Schroeyers, Matthias Auer, Sonja Schreurs. *Application of silver-exchanged zeolite for radioxenon mitigation at fission-based medical isotope production facilities*. Pages 576-588.**


Atmospheric radioxenon releases from fission-based medical isotope production facilities are the main contributors to the radioxenon background being observed in the International Monitoring System (IMS) for the verification of the Comprehensive Nuclear-Test-Ban Treaty. This background is impacting the detection capability of the IMS network for potential nuclear explosions. Reducing the radioxenon emissions from these facilities requires the optimization of the corresponding filtration process. The investigation of more efficient Xe adsorption materials than Activated Carbon (AC), which is currently used for this application, can play an important role for such an optimization. In this work, the Xe adsorption capacity of silver-exchanged zeolites (AgZs) is compared to the one of ACs in relevant conditions for fission-based medical isotope production facilities. The most promising AgZ candidate, a silver-exchanged titanosilicate (Ag-ETS-10), is investigated in more detail for its application to further reduce radioxenon releases. As operational conditions depend on the production and off-gas treatment processes, the effect of Xe concentration, flow rate, temperature and moisture on the Xe adsorption in Ag-ETS-10 is reported. Furthermore, since AgZs are far more expensive than ACs, it is crucial to be able to regenerate the material, whilst maintaining its full Xe adsorption properties for successive reuse. Accordingly, the durability of Ag-ETS-10 is investigated with regard to desorption and adsorption cycles but also with regard to gamma irradiation.



- **Keywords:** Xenon adsorption; Regeneration; Silver-exchanged zeolite; Activated carbon; CTBT verification; Medical isotope production facilities


**Vahid Vatanpour, Ehsan Shokouhifar, Azim Ziyaei Halimehjani, Tao He. *Impact of dithiocarbamate-based polymeric additives on the performance of polyethersulfone membrane for the treatment of arsenic contaminated waters*. Pages 589-606.**


Two types of aliphatic and aromatic dithiocarbamate (DTC) polymers, having the thioamide groups were synthesized and used as hydrophilic agents as well as arsenic adsorbents in fabrication and modification of polyethersulfone (PES) membranes for the separation of arsenic from the contaminated water. The synthesized DTCs were characterized by nuclear magnetic resonance (NMR) and Fourier transform infrared spectroscopy (FTIR), and their arsenic adsorption test demonstrated arsenic removal of 85.5% and 91.4% for the aromatic and aliphatic DTC polymers respectively. The results indicated that by increasing the concentration of DTCs, both membrane flux and rate of arsenic removal increased compared to the bare one. The water flux reached a maximum value at 0.5 wt% DTCs and further increase lead to decreased flux. The aliphatic DTC behaved better than the aromatic one: the membrane with aromatic DTC showed better arsenic rejection than the aliphatic one, corresponding well to the adsorption results. The water contact angle was reduced by the addition of DTCs, indicating increased hydrophilicity. The fouling resistance increased by the addition of DTCs which was demonstrated by increased flux recovery ratio (FRR) after BSA fouling. The real arsenic polluted groundwater treatment for a long-time showed that tailored-made DTC polymers

are excellent candidates for arsenic removal and improvement for the fouling resistance of PES membranes.


- **Keywords:** Membranes; Polymeric additives; Dithiocarbamate; Arsenic removal; Fouling reduction


### Hayri Yaman. *Investigation of the effect of compression ratio on the energetic and exergetic performance of a CI engine operating with safflower oil methyl ester*. Pages 607-624.


This study examines the energy and exergy analyses for a single-cylinder, four-stroke, direct-injection, compression-ignition (CI) engine when it was run on the safflower (Carthamus tinctorius L.) oil methyl ester (SOME) and traditional diesel (as reference fuel) at various engine loading conditions (from 25% to full load in 25% steps) at a fixed speed of 1500 rpm. In addition, the compression ratio (CR) was changed between 12:1 and 18:1 in order to monitor its effect on the engine characteristics. The experimental outcomes obtained from the above-stated analyses showed that the tested engine spent more alternating fuel because of its lower energy content than that of diesel fuel in an effort to ensure the output power to be the same for the test fuels. Furthermore, the results exhibited that the energetic and exergetic efficiency enhanced with the increase of load and CR. In this contest, at the CR of 18:1 and full load, the maximum energy efficiency values for SOME and diesel fuel were found to be 28.67% and 29.78%, respectively meanwhile the related exergetic efficiency values were calculated to be 26.41% and 27.94%, respectively. The minimum exergy destruction figures were revealed at the CR of 18:1 and a load of 100% for tested fuels with the findings of 56.59% for SOME and 55.22% for diesel fuel. In conclusion, the results of the conducted analyses for the tested diesel engine powered by SOME appeared to be fairly close to those of diesel fuel at various loads and CRs. SOME will eventually be classified as an alternate fuel to petroleum-based diesel fuel.



- **Keywords:** Alternative fuel; Compression ratio; Energy and exergy analyses; Exergy destruction, Sustainability index


### Rahat Alam, Saif Ullah Khan, Muhammad Usman, Mohammad Asif, Izharul Haq Farooqi. *A critical review on treatment of saline wastewater with emphasis on electrochemical based approaches*. Pages 625-643.


Increasing discharge of saline wastewater (SWW) from different industries and environmental risks associated with it has compelled researchers to search for efficient treatment methods and safe disposal techniques. Unfortunately, several industries such as agro-food, oil & gas, tannery, and pulp & paper require brine solution units to obtain a finished product that further elevates the salinity of discharged wastewater to a magnitude of 1–3% by weight of NaCl. Among the conventional treatment procedures, electrochemical technologies proved to be more efficient, robust and cost-effective. Electrocoagulation (EC), an electrochemical based technology that produces in situ coagulant which ultimately assist in pollutant removal. It is even more suitable for the treatment of saline water as salinity increases conductivity which further enhances the EC process efficiency. However, the elevated anodic dissolution may increase the cost which can be reduced by using scrap metals as sacrificial electrodes out of iron and aluminum. The mechanism of salt removal from SWW using EC is similar to other pollutant removal mechanisms as salt species being coagulated by the metal hydroxides and are further removed as sludge. However, optimization of process parameters in EC is essential to maintain a balance between anodic passivation and higher metal dissolution so as to make the process efficient. This review paper highlights the theory of the EC technology, process parameters, potential application and recent developments of EC for the treatment of various types of SWW as well as economical assessment associated with this technology. Most of the recent research concerning EC for SWW treatment has been

concentrated on the pollutant-specific evaluation without paying special attention to the process optimization, process modeling and commercial usage. This review further outlines the challenges with the recommendations for encouraging research options that can potentially enhance the EC performance, lower the operational costs and expand its range of applications for SWW treatment.

- **Keywords:** Salinity; Electrocoagulation; Conductivity; Hydroxide precipitation; Energy consumption

**Ji Ge, Yuyuan Zhang, Kaili Xu, Jishuo Li, Xiwen Yao, Chunying Wu, Shuangyuan Li, Fang Yan, Jinjia Zhang, Qingwei Xu. *A new accident causation theory based on systems thinking and its systemic accident analysis method of work systems*. Pages 644-660.**

Major accidents such as the Space Shuttle Challenger disaster in the USA, the Bhopal Disaster in India, the Fukushima nuclear accident in Japan, and the Tianjin Port fire and explosion accident in China, have occurred all over the world. Safety scientists are always trying to understand why these accidents happened and how to prevent these accidents. Accident models and theories form the basis for many safety research fields and practices. However, there is no universally accepted model with useful elements relating to understanding accident causation, although many accident causation models exist. A new accident causation theory named the Interaction Theory of Hazard-Target System (ITHTS) is proposed based on Systems-Theoretic Accident Model and Processes (STAMP) and Risk Management Framework (RMF), which not only incorporates human, organisational and technological characteristics in the same framework, but also considers the sociological factors such as legislative, regulatory, and cultural factors. On the other hand, a new systemic accident analysis method of work systems (SAAMWS) is proposed based on ITHTS and STAMP because ITHTS cannot be applied directly in accident analysis. We choose Tianjin Port fire and explosion accident as a case study to demonstrate the explanatory power of Interaction Theory of Hazard-target System and the feasibility of the new accident analysis method. Further research needs to be done to assess the reliability and validity of this new systemic accident analysis method.

- **Keywords:** Accident causation model; Risk Management Framework; STAMP; Safety constraint; ITHTS; Systemic accident analysis method

**Dong Chen, Nan Li, Weichen Sun. *Rupture properties and safety assessment of raw coal specimen rupture process under true triaxial hydraulic fracturing based on the source parameters and magnitude*. Pages 661-673.**

To realize the safety assessment and risk management of the raw coal specimen rupture process under true triaxial hydraulic fracturing, the AE parameters and source parameters were obtained based on the AE monitoring of raw coal specimen rupture under true triaxial hydraulic fracturing. Throughout the process of hydraulic fracturing, the variation rule of AE parameters and the spatio-temporal distribution of the AE events induced by hydraulic fracturing of raw coal under true triaxial stress were studied. Then, based on the Brune model and grid search method, the source parameters and moment magnitude of raw coal specimens rupture under true triaxial hydraulic fracturing were obtained, and the relationship between the seismic moment and the other source parameters was analyzed. Finally, the source parameters relating AE events in raw coal specimens rupture under true triaxial hydraulic fracturing and micro-earthquakes induced by hydraulic fracturing were compared and investigated; the relationship between Mw (moment magnitude) and ML (local magnitude) of AE events of raw coal specimens rupture under true triaxial hydraulic fracturing was revealed. The results show that: the AE locating results are generally consistent with the actual rupturing of raw coal

specimens. The source displacement spectrum of raw coal specimens rupture under true triaxial hydraulic fracturing is in good accordance with predictions made using the Brune model. By calculating the source parameters and moment magnitude, the source scale of hydraulic fracturing of raw coal specimens under true triaxial stress can be evaluated accurately. Source parameters such as corner frequency and apparent stress of raw coal specimen decrease linearly with the increase of seismic moment, and the source radius and source energy increase linearly with the increase of seismic moment; the stress drop tends to fluctuate around a certain value. The source properties of hydraulic fracturing of raw coal specimens under true triaxial stress can be evaluated. The seismic source properties relating AE events in raw coal specimens rupture under true triaxial hydraulic fracturing and micro-earthquakes induced by hydraulic fracturing are different. Considering Mw, ML1 can be better used to calculate the magnitude of AE events of raw coal specimens rupture during true triaxial hydraulic fracturing. These results can reveal the source properties throughout the rupturing of raw coal specimens during true triaxial hydraulic fracturing, and evaluate the safety of rupture process.


- **Keywords:** Raw coal specimen; Hydraulic fracturing process; AE parameters; Source parameters; Source properties; Mw and ML, Safety assessment


### Ya Tang, YuTing Xu, BingJian Zhang, Chang He, QingLin Chen, Jingzheng Ren. *An integrated computational strategy for the geometric design and prioritization of wave-plate mist eliminators*. Pages 674-686.

In this study, a computational strategy is proposed for geometric design and prioritization of wave-plate mist eliminators by combining the Taguchi experimental design, CFD modelling, and Fuzzy Analytic Hierarchy Process (FAHP) approaches. The Taguchi approach is first used to identify a balanced set of geometric parameters and to generate 16 design cases depending on the chosen levels. A batch of CFD runs is then performed on these design cases to obtain the detailed multi-phase flow behaviour. Finally, the FAHP approach is employed in assisting the multi-criteria decision-making process of these design cases based on multi-run CFD results. To probe the separation mechanism, five design cases (named Cases 4, 8, 12, 15, and 16) with relatively high graded mean integration representation scores (GMIRs=0.0819, 0.0774, 0.0814, 0.0784, 0.0780) are systematically compared and analyzed regarding the profiles of static pressure, velocity, turbulent kinetic energy, etc. It indicates that Case 4, with the maximum level of bends (n = 4) and dimensionless width (W/S=0.55), as well as the minimum wavelength of a bend (λ = 1), can effectively reduce the power consumption while achieving a higher separation efficiency.


- **Keywords:** Wave-plate mist eliminator; Prioritization; Taguchi experimental design; Fuzzy Analytic Hierarchy Process; Power consumption; Separation efficiency


### Wenshi Liu, Kai Xiao, Jing Li, Jin Zhu, Lingru Sun, Changtao Chen. *Efficient removal of organic contaminants in real shale gas flowback water using Fenton oxidation assisted by UV irradiation: Feasibility study and process optimization*. Pages 687-697.

The aim of this study was to identify an effective method for removing organic pollutants from real shale gas flowback water (SGFW). The results showed that ozonation could only achieve limited total organic carbon (TOC) removal when the initial pH was set to 3 or 7. Compared with the O3/H2O2 and Fenton processes, better performance was observed with the ultra violet (UV)-Fenton process in SGFW. The effects of H2O2/COD, initial pH, H2O2/Fe2+, and reaction time on the removal efficiency via the UV-Fenton process were investigated through single-factor experiments. The optimal experimental conditions were obtained using a quadratic polynomial prediction model (RAdj2 = 0.9295)

from the central composite design of response surface methodology. The TOC removal efficiency could reach as high as 70.02% even in real SGFW under optimal conditions (H2O2/chemical oxygen demand ratio 11.54, H2O2/Fe2+ ratio 130.20, pH 3.72, temperature 25 °C, and reaction time 60 min). Moreover, the TOC removal kinetics could be better explained by pseudo-second-order kinetics (R2=0.9609). In UV-assisted Fenton oxidation, the cycle of Fe3+ species to Fe2+ was accelerated to regenerate more ·OH radicals, thereby leading to higher TOC removal efficiency. Moreover, gas chromatography-mass spectrometry analysis revealed that the UV-Fenton process could mineralize most organic pollutants in the SGFW. Dibutyl phthalate was selected as the model organic matter to explore the possible degradation mechanism. This study provides a reference for the design and operation of organic removal units in the SGFW treatment process.

- **Keywords:** Shale gas; Flowback water; UV-Fenton; Hydroxyl radical; Response surface methodology; Dibutyl phthalate

**Sifeng Jing, Xiwei Liu, Xiaoyan Gong, Ying Tang, Gang Xiong, Sheng Liu, Shuguang. Xiang, Rongshan. Bi. *Correlation analysis and text classification of chemical accident cases based on word embedding*. Pages 698-710.**

Accident precursors can provide valuable clues for risk assessment and risk warning. Trends such as the main characteristics, common causes, and high-frequency types of chemical accidents can provide references for formulating safety-management strategies. However, such information is usually documented in unstructured or semistructured free text related to chemical accident cases, and it can be costly to manually extract the information. Recently, text-mining methods based on deep learning have been shown to be very effective. This study, therefore, developed a text-mining method for chemical accident cases based on word embedding and deep learning. First, the word2vec model was used to obtain word vectors from a text corpus of chemical accident cases. Then, a bidirectional long short-term memory (LSTM) model with an attention mechanism was constructed to classify the types and causes of Chinese chemical accident cases. The case studies revealed the following results: 1) Common trends in chemical accidents (e.g., characteristics, causes, high-frequency types) could be obtained through correlation analysis based on word embedding; 2) The developed text-classification model could classify different types of accidents as fires, explosions, poisoning, and others, and the average p (73.1%) and r (72.5%) of the model achieved ideal performance for Chinese text classification; 3) The developed text-classification model could classify the causes of accidents as personal unsafe act, personal habitual behavior, unsafe conditions of equipment or materials and vulnerabilities management strategy; p and r were 63.6% for the causes of vulnerabilities management strategy, and the average p and r are both 60.7%; 4) the accident precursors of explosion, fire, and poisoning were obtained through correlation analyses of each high-frequency type of chemical accident case based on text classification; 5) the text-mining method can provide site managers with an efficient tool for extracting useful insights from chemical accident cases based on word embedding and deep learning.

- **Keywords:** Text mining; Correlation analysis; Text classification; Word embedding; Deep learning; Chemical accident cases

**Pengjie Liu, Huanli Sun, Yantao Qiao, Shijie Sun, Chengdong Wang, Kaiqiang Jin, Binbin Mao, Qingsong Wang. *Experimental study on the thermal runaway and fire behavior of LiNi0.8Co0.1Mn0.1O2 battery in open and confined spaces*. Pages 711-726.**

With the increasing deployment of large-scale lithium ion batteries (LIBs), thermal runaway (TR) and fire behavior are significant potential risks, especially for high energy density cells. A series of thermal abuse tests and hazard analysis on 117 Ah LiNi0.8Co0.1Mn0.1O2/graphite LIBs were performed under two conditions, "open space" and "confined space". In open space tests, the fire behavior of LIBs was characterized with respect to the TR process, temperature characteristics, mass variation, voltage, heat release rate and gas release. To simulate the application scenarios in electric vehicles, a confined cabinet was introduced. The effects of state of charge and confined cabinet on the fire behavior of individual cell were analyzed. Furthermore, a real-scale scenario was considered for the evaluation of fire-induced toxicity using Fractional Effective Dose (FED) and Fractional Effective Concentration (FEC) models. The obtained results show that the effects of asphyxiant gases are more significant than those of irritant gases. The maximum FEC and FED values are greater than the critical threshold of 1, indicating the catastrophic toxicity in such fire scenarios. The minimum fresh air renewal rate required is computed to provide quantitative guides for ventilation management, firefighting and rescue.

- **Keywords:** Lithium ion battery safety; LiNi0.8Co0.1Mn0.1O2 cell; Thermal runaway; Fire behavior; Gas release