# Process Safety and Environmental Protection

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**Guohui Li, Kang Chen, Hong Yang. *A new hybrid prediction model of cumulative COVID-19 confirmed data*. Pages 1-19.**

Establishing an accurate and efficient prediction model is of great significance for governments and other social organizations to formulate prevention and control policies and curb the explosive spread of the pandemic. To improve prediction accuracy of cumulative COVID-19 confirmed data, a new hybrid prediction model based on gradient-based optimizer variational mode decomposition (GVMD), extreme learning machine (ELM), and autoregressive integrated moving average (ARIMA), named GVMD-ELM-ARIMA, is proposed. To solve the problem of selecting the k value and the penalty factor α in variational mode decomposition (VMD), this paper proposes gradient-based optimizer variational mode decomposition (GVMD), which realizes the self-adaptive determination of k value and α value. Firstly, GVMD decomposes the cumulative COVID-19 confirmed data into some intrinsic mode functions (IMFs) and a residual component (IMFr). Secondly, IMFs are predicted by ELM. Then, IMFr is predicted by ARIMA. Finally, the final prediction results are obtained by reconstructing the prediction result of IMFs and IMFr. The cumulative COVID-19 confirmed data of the United States, India and Russia is used to verify its effectiveness. Taking the United States as an example, compared with the average MAPE, RMSE and MAE of the single model, the average MAPE of the hybrid model is reduced by 47.27%, the average RMSE is reduced by 44.50%, and the average MAE is reduced by 55.34%. Compared with GVMD-ELM-ELM, GVMD-ELM-ARIMA proposed in this paper reduces the MAPE by 60%, the RMSE by 56.85%, and the MAE by 61.61%. The experimental results show that GVMD-ELM-ARIMA has best prediction accuracy, and it provides a new method for predicting the cumulative COVID-19 confirmed data.

- **Keywords:** COVID-19; Cumulative confirmed data; Prediction; Variational mode decomposition

**Jiao Du, Xiaoxian Shang, Tao Li, Yueping Guan. *Recycling and modeling of chromium from sludge produced from magnetic flocculation treatment of chromium-containing wastewater*. Pages 20-26.**

In this paper, an effective and sustainable treatment method for recycling chromium from sludge produced by magnetic flocculation was established. Chromium was extracted from sludge with hydrogen peroxide and sodium hypochlorite, and then, superparamagnetic ferroferric oxide nanoparticles (MPs) were recovered by magnetic separation. The recovery percentage of chromium with sodium hypochlorite was higher

than that with hydrogen peroxide, and the maximum was 99.12%. With increasing MPs use times, the adsorption percentage of chromium decreased, but there was no significant change in the recovery percentage of chromium in sludge. The purity of the recovered sodium chromate crystals was 96.28%. The back-propagation algorithm was used to model chromium recovery. The correlation coefficient between the model prediction data and experimental data was 0.9990, and the average absolute error was 0.51. The maximum recovery percentage of chromium obtained from model prediction was 99.27%, and the corresponding optimal conditions were consistent with those of experiments.


- **Keywords:** Chromium-containing sludge; Chromium recovery; Tanning wastewater; Magnetic particles; Artificial neural network; Back-propagation


### Pingjie Fu, Keming Yang, Fei Meng, Wei Zhang, Yu Cui, Feisheng Feng, Guobiao Yao. *A new three-band spectral and metal element index for estimating soil arsenic content around the mining area*. Pages 27-36.


Owing to the advantages of fast and non-destructive measurement, visible and near-infrared reflectance (VNIR) spectra have been widely used in the study of heavy metal pollution. However, few studies have focused on the estimation of soil heavy metal concentration by the enhanced joint architecture of spectral indices and metal elements enriched in clay minerals. In this work, a new composite index, namely Three-band Spectral and Metal Element Index (TSMEI), is proposed to retrieve arsenic (As) in soil by utilizing the multi-view spectral information. Based on obtained data, including spectra and the concentration of iron (Fe), potassium (K), aluminum (Al), magnesium (Mg) and arsenic (As) of the soil around the open-pit coal mine area, the three-band spectral index (TBSI) for As, K, Fe, Mg and Al were calculated from four types of spectral data, that is, raw reflectance (R), the first-order derivative of the spectrum (FD), spectral continuum removal (CR) and spectral reciprocal logarithmic (RL). Then, the metal element index (MEI) for As concentration were constructed via estimated content of K, Fe, Mg and Al based on their TBSIs. Finally, the optimized TBSIs and MEIs were used to construct TSMEI, and it was combined with random forest to invert the As concentration. The following conclusions are drawn: TBSIs is significantly better than that dual-band spectral index and single-band spectrum for estimating As content, and the correlations between the TBSIs based on the FD and the As concentration perform best ($r \geq 0.7684$). In addition, two/three element MEIs show higher correlation coefficients with As concentration compared to individual metal element. Furthermore, the proposed TSMEI allow high-precision estimation of As content, which acquired highest correlation coefficient and lowest RMSE ($r = 0.9732$, RMSE = 0.0703). The results confirm that the TSMEI is significantly effective in estimating soil As content.



- **Keywords:** Hyperspectral data; Soil heavy metal; Mining area; Spectral index; Metal element index


### Joshua O. Ighalo, Setyo Budi Kurniawan, Kingsley O. Iwuozor, Chukwunonso O. Aniagor, Oluwaseun J. Ajala, Stephen N. Oba, Felicitas U. Iwuchukwu, Shabnam Ahmadi, Chinenye Adaobi Igwegbe. *A review of treatment technologies for the mitigation of the toxic environmental effects of acid mine drainage (AMD)*. Pages 37-58.


Acid mine drainage (AMD) is a multi-factor pollution formed from complex chemical, physical, and biological interactions that takes place under ambient conditions in abandoned and active mines. Over the years, researchers have been investigating ways to mitigate its potential impact on the environment through various treatment technologies. The aim of this review was to critically analyze the broad spectrum of treatment methods that have been engaged in published literature on the remediation of

AMDs. Adsorption treatment using zeolites, fly ash, biochar activated carbon, clay-based minerals and biomass-based adsorbents was discussed. Given an appropriate choice of adsorbent, ions in AMD can be reduced between 50% and 99%. Membrane separation processes like nanofiltration, reverse osmosis and hybrid systems were discovered to be more effective than adsorption and can effect over 90% rejection at optimized conditions. Biological processes showed a far wider range of performance amongst all treatment types due to the selectivity in performance of the different micro-organisms used although Advanced Oxidation Process (AOPs) have been shown to achieve>80% ions removal. In all biological processes studied ranging from wetlands to bioreactors, algal bioreactors seemed the most effective in this domain. Most of these treatment technologies are corrective while preventive techniques can be explored to prevent the production of AMD. Despite the positive outcomes of the different types of treatment, they have associated technical issues. It is recommended that more preventive techniques be explored to reduce the production of AMD. The review discussed how AMD treatment would affect environmental protection and water resource management.


- **Keywords:** acid mine drainage; ecotoxicology; biological processes; advanced oxidation processes; separation processes


**Puhazhendi Puhazhselvan, Ajitha Pandi, Parthasarathy Baskaran Sujiritha, George Sebastian Antony, Sellamuthu Nagappan Jaisankar, Niraikulam Ayyadurai, Palanivel Saravanan, Numbi Ramudu Kamini. *Recycling of tannery fleshing waste by a two step process for preparation of retanning agent*. Pages 59-67.**


Discharge of huge quantities of fleshing wastes by leather industries has raised serious concerns on account of their environmental impacts. Limed fleshings, a hazardous solid waste produced from leather making process is rich in proteins and lipids. Currently, fleshing waste is not properly utilized and disposed off in unsecured manner. Utilization of fleshings for preparation of value added chemicals provide practically feasible and economically viable solution. This study investigates the feasibility of using fleshings as resource material for preparation of retanning agent by a two step process aiming at recycling of the waste. The fleshings was initially hydrolysed using Bacillus subtilis protease followed by polymerization with methacrylic acid. The performance of the resulting fleshings hydrolysate-acrylic polymer (FHAP) was assessed as retanning agent. The FHAP treated leather exhibited better fullness, grain tightness and smoothness than control leather and also improved the strength properties of the leather. SEM results revealed that the treated leather showed more cemented fiber bundles due to the efficient filling of interfibrillar space of the leather, which was confirmed by air permeability analysis. Thus, preparation of FHAP for retanning application offers sustainable solution to the problem of fleshing waste management and also an appropriate strategy for circular economy.



- **Keywords:** Circular economy; Fleshing waste; Leather; Protease; Protein acrylic polymer; Retanning agent


**Senem Yazici Guvenc, Emine Can-Güven, Gamze Varank. *Persulfate enhanced electrocoagulation of paint production industry wastewater: Process optimization, energy consumption, and sludge analysis*. Pages 68-80.**


This study aimed to investigate the treatment of paint production industry (PPI) wastewater, which is characterized by low biodegradability and high concentrations of resistant organic matter, by persulfate enhanced electrocoagulation process (EC-PS). A regression quadratic model was developed to describe the removal of chemical oxygen demand (COD) and color number (CN) from PPI wastewater. The effects of independent

variables (initial pH, PS dose, current density, and reaction time) on system responses and the interaction between the parameters were determined. Validation experiments were carried out under the optimum conditions determined by the quadratic model (initial pH: 5, PS dose: 5.6 g/L, current density: 21 mA/cm2, and reaction time: 35 min) and 64% COD and 98.1% CN removal were obtained. Pollutant removal efficiencies increased with the increase of PS dose, current density, and reaction time while the highest removal efficiencies were achieved at acidic pH values. The scavenging studies indicated that although the sulfate radicals were the dominant radical type, both hydroxyl and sulfate radicals were involved in the process. In the synergistic effect studies performed under optimum conditions, the highest reaction rate was obtained in the EC-PS process with a value of 0.074 1/min. Specific energy consumption under optimum conditions was calculated as 20.4 kWh/kg COD. The results of the study showed that the EC-PS is an effective process for the treatment of PPI wastewater and response surface methodology is an applicable technique for the optimization of the variables.


- **Keywords:** Color number; Box-Behnken design; Electrocoagulation; Paint production industry wastewater; Persulfate


### Miaomiao Zhao, Degang Ma, Qiji Wang, Yuxin Wang, Xianfu Sun. *Electrokinetic remediation of Cd-contaminated soil using low voltage gradients coupled with array adsorption zone and polarity Exchange*. Pages 81-91.


Soil Cd pollution is a threat to the global ecological environment. Electrokinetic remediation (EKR) generally uses strong electric fields to obtain high removal efficiency, which leads to a series of side reactions and high energy consumption. EKR using low-voltage gradients showed weak migration of Cd and low remediation efficiency. Herein, to develop an effective enhanced EKR technology using low voltage gradient (0.2 V·cm−1), array adsorption zone and polarity exchange were applied simultaneously. Five experiments were conducted to determine the effect of polarity exchange, array adsorption zone and their combination on Cd removal when EKR was carried out at 0.2 V·cm−1. Results showed that the combined use of the array adsorption zone and polarity exchange achieved optimal remediation and average Cd removal efficiency was 83%. Moreover, the reciprocating motion of Cd caused by polarity exchange is no longer a side effect. In the wheat cultivation experiment, the Cd concentration of wheat root, stem and leaf decreased by 86%, 93% and 95% after Cd was removed by EKR coupled with array adsorption zone and polarity exchange. The 30-day energy consumption is 7.72 kWh·m−3, which is far lower than that of other enhancement methods. The present work proposes an effective EKR technology working at low voltage for Cd-contaminated soil.



- **Keywords:** Electrokinetic remediation; Array adsorption zone; Polarity exchange; Cadmium-contaminated soil


### Eunji Shin, Sangwoo Yoo, Yongtaek Ju, Dongil Shin. *Knowledge graph embedding and reasoning for real-time analytics support of chemical diagnosis from exposure symptoms*. Pages 92-105.


Chemical exposure accidents pose a risk of serious injury and property damage if the diagnosis or response is not properly performed after the initial discovery. Due to lack of research on the dynamically changing environment and detection of chemical substances considering symptoms, real-time knowledge services are required, such as rapid diagnosis of chemicals exposed at the accident site and the following early response. In this study, we propose an AI-based analysis system, Symptom-based Expert for Advanced Response to Chemical Hazards (SEARCH), for chemical substance diagnosis from exposure symptoms actively collected for real-time response and mitigation to

hazardous material accidents. Knowledge is collected from chemical database such as WISER, PubChem etc., and integrated for the analytics of chemical exposure accidents and contact symptoms. We design and construct ontology and knowledge graph (KG) for 1001 major chemical substances. The built KG is verified using KG embedding models and the performance of each model is compared. The proposed system identifies the substance candidates through KG query and reasoning considering the exposure conditions. Using the symptom KG, the system SEARCH can provide the means to analyze real-time data from the field and transform it into insights and actions related to emergency response.


- **Keywords:** Chemical Safety; Exposure Symptom Knowledge; Data Analytics; Knowledge Graph; Knowledge Graph Embedding; Knowledge Graph Reasoning


### Sultan K. Alharbi, Ashley J. Ansari, Long D. Nghiem, William E. Price. *New transformation products from ozonation and photolysis of diclofenac in the aqueous phase*. Pages 106-114.


Ozone and UV photolysis can be effective for the treatment of pharmaceuticals in wastewater, however, these processes can result in the formation of potentially toxic transformation products (TPs). This study investigates the structural elucidation of the TPs formed during ozone and UV treatments of diclofenac (DCF), a ubiquitous pharmaceutical. Using liquid chromatography – electrospray ionisation - mass spectrometer (LC-ESI-MS) and a Waters Xevo™ Quadrupole Time-of-Flight (Qtof) mass spectrometer, the chemical structures of DCF TPs were identified, including the fragmentation ion patterns and exact mass of the detected molecular ions. TPs formed during ozonation showed an addition of one or more hydroxyl groups to the DCF molecule including changes to the double bond equivalent for some products. The other identified DCF ozonation products were formed by removal of the (-CH2COOH) group in two steps and resulted in the formation of a diverse range of TPs. By contrast, UV photolysis formed DCF TPs via removal of its chlorine atoms and ring closure followed by dimerization. In comparison, all ozonation TPs retained the two chlorine atoms of DCF whereas UV TPs did not possess any chlorine atom except for one compound that retained one chlorine atom. Possible reaction pathways for the identified DCF TPs are also proposed.



- **Keywords:** Diclofenac (DCF); Oxidation; Transformation products; Ozonation; UV photolysis; Reaction mechanisms


### Qianqian Xue, Wen Nie, Lidian Guo, Qiang Liu, Yun Hua, Ning Sun, Chengyi Liu, Wenjin Niu. *Determining the optimal airflow rate to minimize air pollution in tunnels*. Pages 115-130.


With the spreading of the green environmental protection concept, increasing attention has been paid to improving the tunneling environment. In this paper, the distribution characteristics of airflow fields, the diffusion laws of pollutants, and the influence of airflow rate changes on pollutants in tunnels under single-forced ventilation conditions were simulated according to the computational fluid dynamics (CFD) theory. In addition, the reliability of the simulation results was verified through field measurements. A three-stage distribution was observed once the dust concentration stabilized: we noticed areas with relatively low dust concentrations (<300 mg/m3), high dust concentrations (>500 mg/m3), and medium dust concentrations (~400 mg/m3, near the tunnel exit). Meanwhile, after stabilizing, the gas concentration was 0.67%. Properly increasing the airflow rate (Q) can effectively improve the tunnel environment: when Q reached 600 m3/min, the air in the tunnel was effectively purified. However, under a continuous increase of the airflow rate, there is a risk of pollution rebound.We conclude that, to effectively improve the tunnel environment and achieve a sustainable utilization of resources, the optimal operation airflow rate should be 600 m3/min.

- **Keywords:** Temporal–spatial evolution law; Dust and gas two-phase migration coupling; Optimal blowdown air rate; CFD simulation; Tunnel environment optimization

**Xiangyu Zhao, Kuang Cheng, Wang Zhou, Yi Cao, Shuang-hua Yang, Jianmeng Chen. *Source term estimation with deficient sensors: A temporal augment approach.* Pages 131-139.**

Air pollution of chemical industrial parks (CIPs) is becoming increasingly severe, which has major impacts on the health of local residents. Therefore, source term estimation (STE) is of high importance to find the source locations and back-calculate the source emission rates based on the ambient concentration measurements and meteorological information. However, the number of the ambient sensors is far less than the one of pollution sources for CIPs. This issue of sensor deficiency makes the unknown source parameters untraceable. In this paper, the concept of traceability is introduced to propose a condition to explain when the STE problem has a unique solution. Then an approach using measurements at multiple time points for estimating the emission rate of each source is proposed. In order to satisfy the condition of traceability, the coefficient matrix can be expanded by augmenting measurement samples collected at different time instances with different wind directions when the emission rates keep unchanged. Furthermore, based on the rank of the coefficient matrix, the problem can be classified as fully traceable, partially traceable, and untraceable. Then, the regularized least squares method is applied to estimate the source rates in real-time. Some test results with a simulated scenario demonstrate that the source rate can be reliably estimated with the method proposed. Finally, the limitations and conclusions of the method are stated.

- **Keywords:** Air pollution; Chemical industrial park; Source term estimation; Traceability; Regularized least squares solutions

**Bor-Yih Yu, Ting-Yu Tseng, Zhen-Yu Yang, Shiau-Jeng Shen. *Evaluation on the solketal production processes: Rigorous design, optimization, environmental analysis, and control*. Pages 140-155.**

This works aims at evaluating different process configurations for producing solketal from reacting glycerol with acetone. The research carries out the regression of thermodynamic and kinetic parameters, rigorous design of four process configurations, optimization, carbon emission analysis, and control. The results from steady-state analysis reveal that the solvent-free coupled reaction/distillation (SFCRD) process is the most promising. It reduces 40.09% of total annual cost and 45.09% of CO2 emission from the base case, the separated reactor-distillation process. Besides, the CO2 emission rate of the SFCRD process is found 35.29% and 65.91% less than the recently reported upper and the middle partition reactive dividing-wall column process, respectively, indicating the unfavorability of intensifying this reacting system through reactive distillation. Finally, a control structure for the SFCRD process is established for effectively handling the disturbances from the flowrate, composition and catalyst deactivation. Through the dynamic simulation, the closed-loop control results were revealed satisfactory.

- **Keywords:** glycerol; solketal; process design; simulated annealing; coupled reaction/distillation; carbon emission

**Jiajia Xu, Qiangling Duan, Lin Zhang, Yujun Liu, Chunpeng Zhao, Qingsong Wang. *Experimental study of the cooling effect of water mist on 18650 lithium-ion battery at different initial temperatures*. Pages 156-166.**

The depletion of fossil fuels has led to the rapid development of environmentally friendly lithium ion battery (LIB). However, exposure of LIB to elevated temperatures frequently leads to battery failure, thermal runaway (TR), or even TR propagation. In this study, a series of experiments are conducted on the LIBs with and without water mist at different initial temperatures (50 °C and 106–206 °C) in a novel designed battery module to investigate the cooling effect of water mist. The results show that water mist reduces the possibility of battery failure and inhibits TR. The critical temperature of TR is enhanced by 36 °C. Moreover, using water mist to suppress the TR propagation requires reducing the temperature of a cell that undergoing TR to below 126 °C. Analysis of cooling rate indicates that there are four cooling modes ((Ⅰ) rapid cooling and quasi-steady state, (Ⅱ) rapid cooling and slow cooling, (Ⅲ) transitional stage, and (Ⅳ) rapid heating and rapid cooling) of water mist. The heat absorbed by water mist is distinct in four cooling modes. These results reveal that water mist has better cooling effect and the cooling mode changes with the increase of temperature, which may provide insight into the thermal safety performance of cells.


- **Keywords:** Lithium ion battery safety; Cooling effect; Water mist; Thermal runaway


### Shichun Weng, Wenqian Wu, Zichao Guo, Fuqing Meng, Ying Chen, Wanghua Chen. *The formation mechanism and thermal decomposition kinetics of 2,4,6-trinitroresorcinol in the dinitrobenzene production*. Pages 167-174.

2,4,6-Trinitroresorcinol (TNR), one main by-product in the dinitrobenzene (DNB) production process, is self-reactive substance and has led to tragic explosion incidents in China. In this article, the formation mechanism of TNR during the DNB production process was studied employing HPLC and HPLC-MS technique. Thermal decomposition behavior of TNR was also systematically studied by differential scanning calorimeter (DSC). The decomposition kinetics of TNR were investigated employing both iso-conversional (Friedman and Ozawa method) and model-fitting method. The formation mechanism of TNR during the dinitrobenzene (DNB) production is confirmed: The two by-products of dinitrophenol (DNP) and trinitrophenol (TNP) produced in the benzene mononitration stage are further nitrated to form tetranitrophenol (TTNP) in the mononitrobenzene (MNB) nitration stage. Then most of TTNP will be hydrolyzed to form the TNR during the water washing process. The decomposition process of TNR has been proven to follow three consecutive steps (A→B1→B2→B). The former two steps present autocatalytic behavior while the last step obeys N-order reaction model. The accuracy of the developed decomposition model and the obtained model parameters have been demonstrated by the comparison of the simulated and experimental DSC data and the activation energy obtained by both the iso-conversional method and model-fitting method. The same trend of experimental and simulated results about isothermal reaction further verify the building model.


- **Keywords:** 2,4,6-Trinitroresorcinol; Nitration; Thermal decomposition; Autocatalysis; Formation mechanism; Tetranitrophenol


### Jinqiu Hu, Chuangang Chen, Zeyu Liu. *Early warning method for overseas natural gas pipeline accidents based on FDOOBN under severe environmental conditions*. Pages 175-192.

The completion and operation of transnational long-distance oil and gas pipelines will not only alleviate shortages of oil and gas resources in China, but also lead to new development opportunities in the countries along their routes. However, the frequent occurrence of severe environmental disasters has led to several uncertainties regarding the long-term safe and stable operation of overseas pipelines, including pipeline fracture,

fire, explosions, etc. In this paper, the fuzzy dynamic object-oriented Bayesian network (FDOOBN) theory was introduced to establish an early warning method for overseas natural gas pipeline accidents under harsh environmental conditions. Firstly, for the harsh environmental conditions (lightning, rain, and wind) at pipeline laying stations, accident scenarios under a single harsh environmental condition and the combination of multiple harsh environmental conditions were constructed. The object-oriented concept was adopted to modularize the station system and equipment, and the dynamic Bayesian network (DBN) model of each subsystem of the station was established. Then, the conditional probability parameters in the model were determined by the fuzzy mathematical method. The DBN model of each subsystem and the dynamic object-oriented Bayesian network (DOOBN) model of the entire station system based on the process flow of the station and the object-oriented concept were introduced in turn to establish the fuzzy dynamic Bayesian network (FDBN) model and the FDOOBN model respectively. The dynamic early warning system for station risk under harsh environmental conditions was finally realized. Finally, the prediction errors of environmental parameters, such as meteorological conditions, were introduced to modify the reliability of the model. The results show that compared with the traditional model, the error-corrected FDOOBN model not only has a better performance in simplifying the modelling process and fully integrating expert experience, but also has an increase in dynamic warning range, further improving the reliability of accident warnings.


- **Keywords:** Overseas pipeline; Fuzzy dynamic object-oriented Bayesian network (FDOOBN); Severe environmental conditions; Early warning


**Bingyu Wang, Jinsong Zhao. *Automatic frequency estimation of contributory factors for confined space accidents*. Pages 193-207.**

Although the dangers of working in confined spaces have been known for many years, fatal accidents related to working in confined spaces still frequently occur. Considerable research has been conducted to identify potential contributory factors of confined space incidents through analyzing accident reports. However, accident databases are usually read and interpreted manually by human experts. The process of analyzing confined space accident reports can be time-consuming and labor-intensive. As the number of accident records increases, it is difficult for the experts to manually review all the reports. Moreover, different individuals may reach various conclusions from the same accident report. Some analysts may fail to capture all the meaningful and relevant causal factors. Automatic information extraction using special rules and ontology-based approaches can be used to mine reports of confined space accidents. However, such approaches tend to suffer from the problem of weak generalization. To overcome this limitation and improve the performance of contributory factors analysis, an improved deep learning based framework is proposed in this paper to automatically extract and classify contributory factors from confined space accident reports using BERT-BiLSTM-CRF and CNN models. Research results suggested that the proposed framework can be used as a feasible method to qualitatively and quantitatively explore the contributory factors of confined space accidents. By analyzing a large quantity of confined space accident reports, the frequency of contributory factors can be estimated automatically. This outcome is helpful to significantly improve the risk assessment quality of confined space works.


- **Keywords:** Confined space; Accident reports; Text-mining; BERT-BiLSTM-CRF; CNN


**Wen-He Wang, Yan Huang, Shao-Yu Hu, Wei Su, Yong Pan, Chi-Min Shu. *Thermal hazards analysis for benzoyl peroxide in the presence of hexanoic acid*. Pages 208-217.**

Benzoyl peroxide (BPO) is a common cross-linking agent and initiator that is widely used in the chemical industry. The instability of a substance may be influenced by the presence of impurities; therefore, the thermal hazard of organic peroxides under contamination has always been a topic of interest. In this study, the effects of hexanoic acid (HAA) on the thermal decomposition of BPO were investigated using differential scanning calorimetry (DSC; 2.0, 4.0, 6.0, 8.0, and 10.0 °C/min) experiments. By using the Kissinger-Akahira-Sunose and Flynn-Wall-Ozawa kinetic models, the progress of the obtained DSC curve was fitted linearly, and the thermokinetic parameters of BPO in the presence of HAA were further calculated. The two apparent activation energy calculations consistently indicated that HAA increased the thermal hazard of BPO. In addition, the Coats-Redfern model was adopted to compute the decomposition mechanism function of each phase of the material, and Gaussian 16 was used to determine the atomic bonding levels between the molecules to discover the thermal decomposition reaction path of BPO under the effect of HAA. The study results can be used as a reference for the loss prevention and control of BPO in practical engineering applications.


- **Keywords:** Organic peroxide; Kinetic model; Thermokinetic parameter; Apparent activation energy; Decomposition mechanism


**Tahir Sultan, Haslinda Zabiri, Muhammad Shahbaz, Abdulhalim Shah Maulud. *Performance evaluation of the fast model predictive control scheme on a CO2 capture plant through absorption/stripping system*. Pages 218-236.**

The Classical Model Predictive Control (CMPC) has the drawback of slow response in complex dynamic systems. In this work, the Fast Model Predictive Control (FMPC), which accelerates the computation time through the fragmental solution of a complex quadratic program (QP), is investigated as a possible alternative to control the standard CO2 capture plant using MEA with various step changes. Aspen PLUS® and MATLAB® a are utilized to implement the control strategy. The study concluded that the FMPC controller has an average settling time of 51.42 s for all step changes, which is 74.8% faster than the CMPC. The average IAE value for FMPC was approximately 0.1307 which is 59 times smaller than the CMPC controller. Additionally, the ISE and ITSE values demonstrated much improved outcomes for the FMPC controller. The offsets for the FMPC are maintained at negligible levels through suitable tunning since offsets are the main hurdle observed when the FMPC controller is implemented on chemical process systems.


- **Keywords:** Classical Model Predictive Control (CMPC); Fast Model Predictive Control (FMPC); CO2 capture; System Identification; Absorption/stripping


**Kun-Hua Liu, Yang Xiao, Hao Zhang, Pan Pang, Chi-Min Shu. *Inhibiting effects of carbonised and oxidised powders treated with ionic liquids on spontaneous combustion*. Pages 237-245.**

The waste of the coal-based activated carbon (CBAC) production process, carbonised powder (CP) and oxidised powder (OP), easily store heat, trigger spontaneous combustion under hot storage conditions, and exhibit strong pyrophoricity. CP and OP pose a serious threat to local environments and inhabitants' health. In this work, the spontaneous combustion of waste materials generated during the preparation of activated carbon in the coal chemical industry was studied, which has been less studied by previous researchers, and the spontaneous combustion was prevented and controlled by ionic liquid (ILs), a new type of environmentally friendly inhibitor. The influence of ILs containing [BMIM]+ ([BMIM][BF4], [BMIM][NO3], and [BMIM][I]) on the spontaneous combustion of CP and OP was studied and quantitatively analysed. The different samples' mass loss at different stages was analysed using thermogravimetry at three heating rates (5.0, 10.0, and 15.0 °C/min). A temperature-programmed experiment was used to

test the inhibiting effect in treated samples. The results indicated that ILs had varying inhibiting effects on the pyrophoricity of samples. The ILs [BMIM][BF4] [BMIM][NO3] [BMIM][I] had, in descending order of percent inhibition, an inhibitory effect on OP; the order for CP inhibition was as follows: [BMIM][NO3]> [BMIM][BF4]> [BMIM][I]. After IL treatment, the maximum, minimum, and average apparent activation energy all increased to varying degrees. At 30–180 °C, the average percent of inhibition of [BMIM][BF4]–Y (OP treated with [BMIM][BF4]) and [BMIM][NO3]–T (CP treated with [BMIM][NO3]) was 20.21% and 7.32%, respectively, and the maximum inhibition percent was 38.53% and 16.13%, respectively.

- **Keywords:** Coal-based activated carbon; Heat storage; Mass loss; Inhibition percent; Apparent activation energy

### Qing Ying Yee, Mimi H. Hassim, Nishanth G. Chemmangattuvalappil, Joon Yoon Ten, Rafeqah Raslan. *Optimization of quality, safety and health aspects in personal care product preservative design*. Pages 246-253.

Personal care products (PCPs) are structured products that are constituted by numerous chemicals ingredients. However, there are several hazardous ingredients in PCPs that may cause exposure to consumers and lead to adverse health impacts. The main contribution of this study is the development of a comprehensive framework for the PCP ingredient design that integrates the safety and health aspects as well as performance aspects simultaneously into computer-aided molecular design (CAMD). Mathematical optimization programming is utilized in this study to generate a list of high quality, poses good safety and health-performance PCP preservative candidates. Furthermore, an index-based safety and health effect assessment is presented in this study. In addition, the exposure assessment of the selected molecule is performed by applying Margin of Exposure. A case study on PCP preservative design is presented. Laboratory experiment is carried out to verify the feasibility of the addition of safer and healthier preservative into the eye cream formulation.

- **Keywords:** Computer-aided molecular design; Safety and health index; Personal care products preservative; Margin of exposure; Eye cream

### Yuzhuo Wang, Yingjie Li, Liguo Yang, Xiaoxu Fan, Leizhe Chu. *Revealing the effects of Ni on sorption-enhanced water-gas shift reaction of CaO for H2 production by density functional theory*. Pages 254-265.

The sorption-enhanced water-gas shift (SE-WGS) reaction promoted by Ni-doped CaO (Ni-CaO) was sufficiently investigated by experiments that only displayed macroscopic results instead of microscopic reaction mechanisms. In this work, density functional theory (DFT) was employed to clarify the mechanisms of SE-WGS reaction which was catalyzed by Ni in the presence of CaO. The SE-WGS reaction only promoted by CaO was used as a comparison to clarify the catalysis of Ni. The analysis of electron differential densities, the partial density of states, and formation energy indicate that Ni causes the higher stability and reactivity of the Ni-CaO model than the CaO model. The Ni promotes the release of H2* by rising the adsorption energy of H2*(−0.05 eV) and retains the efficient CO2 capture with the adsorption energy of −1.56 eV. The transient state calculations indicate the SE-WGS reaction prefers to proceed along with the redox mechanism compared with the carboxyl and formate mechanisms on the Ni-CaO surface. The energy barriers for the CO2* generation, H2* generation and desorption are respectively 0.74, 1.77 and 0.10 eV on the Ni-CaO surface, which are lower than those on the CaO surface. Therefore, Ni helps to improve CO conversion and H2 productivity which is consistent with the previous experimental results.

- **Keywords:** Ni-doped CaO; Sorption-enhanced water-gas shift reaction; Density functional theory; H2 production; CO2 capture

**Yu-liang Liao, Jin-yan Yang. *The release process of Cd on microplastics in a ruminant digestion in-vitro method*. Pages 266-272.**

Microplastics (MPs), polymer particles capable of accumulating heavy metals from ambient medias, have been widely found in agriculture and pasture soils. Through the consumption of MPs in soils, heavy metals adsorbed on MPs can be transported into ruminant digestive guts. To explore the behavior of Cd loaded MPs in ruminant digestive system, we initially established a ruminant digestive in-vitro method (RDM) that simulates the rumination cycle between mouth and rumen to evaluate the release rates of Cd on 4 most commonly used undegradable MPs (PE, PP, PVC, and PS) and a biodegradable MP (PLA). After 120 h of adsorption, the Cd adsorption capabilities by 5 MPs ranged from 0.23 μg/g to 2.45 μg/g. Through RDM, all tested Cd loaded MPs released high proportions of Cd with release rates from 21.5% to 41.8%, where PLA showed the highest Cd release rate. Cadmium was mainly released in rumen and abomasum phases, and the rumination cycle between mouth and rumen can affect the Cd release from MPs. The present study provides a new view on the environmental hazard of heavy metal and MP pollution that their co-exposure to ruminants should be taken into account.

- **Keywords:** Microplastic; Cadmium; Ruminant; In-vitro digestion; Release rate

**Wei Yang, Wenxiao Zhang, Baiquan Lin, Guangyao Si, Jianguo Zhang, Jianli Wang. *Integration of protective mining and underground backfilling for coal and gas outburst control: A case study*. Pages 273-283.**

Mining protective coal seams is an effective approach for coal and gas outburst control, but a large amount of gangue is usually produced when mining a thin protective seam and dealing with the gangue can be a challenging task. In the paper, a novel integrated mining system by extracting two panels simultaneously was demonstrated in the 12th coal mine of the Pingdingshan coalfield: one panel was mined in the thin protective coal seam, and the other one was mined in the protected coal seam. The thickness of the protective seam was only 0.8 m, but the mining height reached 1.8 m, indicating that there was about 1 m thick roof stone being mined. An underground coal preparation plant was built, and the mixture of coal and gangue from the protective panel was sorted underground. The sorted coal was delivered to the surface stockpile, while the waste rock was directly backfilled into the gob of the panel in the protected coal seam. Thus, waste rock did not need to be lifted up to the surface, which can reduce material handing cost and minimise mining footprint on the surface. In order to prevent the migration of pressure relief gas into the working areas of the protective coal seam, the main reasons causing gas exceedance in the upper corner of U-shaped ventilation system were investigated, and then the Y-shaped ventilation system and various gas extraction boreholes were implemented to effectively control the pressure relief gas. Numerical models were developed to assess the effect of applying gob backfilling during the extraction of two panels in parallel. The results show that the gob backfilling can reduce the surface subsidence and horizontal movement, which is very helpful for the protection of ground water and surface infrastructures.

- **Keywords:** Backfill; Protective coal seam; Ventilation; Deep mining; Gas

**Amin Mojiri, John L. Zhou, Mansoureh Nazari V, Shahabaldin Rezania, Hossein Farraji, Mohammadtaghi Vakili. *Biochar enhanced the performance of microalgae/bacteria consortium for insecticides removal from synthetic wastewater*. Pages 284-296.**

The presence of pesticides in aquatic environments has threatened marine food resources, aquaculture, fisheries and human health; therefore, two most used insecticides were removed during this study. Two photobioreactors, including biochar and Chlorella vulgaris/activated sludge (reactor 1), and Chlorella vulgaris/activated sludge (reactor 2) were run to remove chlorpyrifos (CPF) and cypermethrin (CYP). Proteobacteria, Bacteroidetes and Chloroflexi were the dominant phyla of activated sludge. The optimization performance of both reactors was conducted by response surface methods. The performance of first photobioreactor was better than that in the second reactor, achieving abatement of 88.80% CPF and 93.12% CYP, at 69.7 h contact time and 0.32 mg/L initial concentration. The toxicity of CPF and CYP to Chlorella vulgaris was monitored under 0–4 mg/L of insecticide concentrations and 0–72 h contact time. The minimum chlorophyll content (2 mg/L) and protein (16.7%), and maximum growth inhibition (89.7%) were recorded at 4 mg/L insecticides concentration and 72 h contact time. Moreover, molecular docking simulation for catalytic enzyme degradation of Proteobacteria, Bacteroidetes and microalgae was carried out using individual hydrolase enzymes: carboxypeptidase in microalgae, isochorismatase hydrolase in Proteobacteria and alpha-L-arabinofuranosidase in Bacteroidetes. Ligand-binding energy, affinity and dimensions of ligands-binding sites in the enzyme cavity were calculated in each case. Hydrolase is an enzyme group that offers a promising practical application for the degradation of CYP and CPF due to its cavity features. This analysis demonstrated the mode of interaction of ligands with hydrolase enzymes in different species.


- **Keywords:** Biochar; Chlorella vulgaris; Chlorpyrifos; Cypermethrin; Hybrid process


**Qiaoyan Shang, Wenwen Chi, Pengfei Zhang, Yujie Ling, Xiaojuan Liu, Guanwei Cui, Wenge Liu, Xifeng Shi, Bo Tang. *Optimization of Bi2O3/TS-1 preparation and photocatalytic reaction conditions for low concentration Erythromycin wastewater treatment based on artificial neural network*. Pages 297-305.**


At present, it is a challenge to degrade antibiotics of low concentrations in wastewater environment, highly effective and eco-friendly photocatalytic processes were considered promising technologies for this degradation. In this work, Bi2O3-loaded titanium silicalite-1 molecular sieve (Bi2O3/TS-1) composites were prepared and used to degrade low-concentration erythromycin (ERM) in wastewater. The content of active components and the dose of photocatalyst are key operating parameters with major effects on photocatalytic efficiency. The optimal parameters (Bi content and photocatalyst dose) were determined through artificial neural network simulating the relationship between key operating parameters and removal efficiency (RE). The maximum RE (98.02%) was measured under optimal operating parameters (Bi % = 5.5%, catalyst dosage = 0.6 g/L). The effects of water quality parameters (such as pH and ERM concentration) were also studied under optimal experimental conditions. Artificial intelligence was used in this work to achieve optimal control of catalyst preparation and photocatalytic reaction conditions. This study provides a useful strategy for the preparation of nanocatalysts and the practical application of high-efficiency photocatalytic reactions.



- **Keywords:** Bi2O3/TS-1; Erythromycin; Photocatalyst; Z-Scheme; Artificial neural network


**Vahid Aryai, Hassan Baji, Mojtaba Mahmoodian. *Failure assessment of corrosion affected pipeline networks with limited failure data availability*. Pages 306-319.**


Many pipeline networks around the world do not have a failure history. Because of financial reasons or lack of technology, this is a common issue for asset managers in

developing and under-developed countries. In the case of data scarcity, it is not straightforward to assess the risk and reliability of such systems. This research proposes a probabilistic framework for analysing the reliability of corroded pipeline networks with limited failure history availability. To achieve this aim through a comprehensive reliability assessment methodology, state-of-the-art corrosion modeling, component and system failure analysis techniques are utilized. A variety of spatio-temporal reliability assessment methods are employed along with the random-field representation of spatially variable parameters to estimate the failure in a large-scale corrosion affected pipeline network. The applicability of the methodology is evaluated through a case-study of buried pipeline network, and the results are verified with failure history data reported by the industry. The results obtained from the proposed methodology, combined with the cost data provided by asset managers make accurate risk assessment of process/water pipeline possible.


- **Keywords:** Pipeline failure; Corrosion modeling; System reliability; Matrix-based reliability; Data scarcity


### Gang Zhou, Jinjie Duan, Biao Sun, Bin Jing, Yang Kong, Yongliang Zhang, Guanhua Ni, Lulu Sun. *Numerical analysis on pollution law for dust and diesel exhaust particles in multi-ventilation parameter environment of mechanized excavation face*. Pages 320-333.


In order to effectively purify the diesel particulate matter (DPM) emitted by the trackless rubber wheel car in coal mining under the premise of dust control. This paper comprehensively investigated the laws of dust and DPM diffusion under forced ventilation and mixed ventilation and under different air intake volumes of the dust removal fan Q and different distances between the extractive air duct outlet and the head L by means of CFD numerical simulation. The following conclusions were drawn. Under mixed ventilation (Q = 450 m3/min) dominated by forced ventilation, when L= 5 m, the overall control effects on low-concentration dust, high-concentration dust and DPM are the best, with the diffusion distances being 46 m, 62 m and 54 m. Under mixed ventilation (Q=750 m3/min) dominated by exhaust ventilation, when L= 5 m, the overall control effects on low-concentration dust, high-concentration dust and DPM are the best, with the diffusion distances being 23 m, 24 m and 39 m, respectively. Therefore, under the above two air volumes, when L= 5 m, the best control effects can be achieved on dust and DPM in the working face.



- **Keywords:** Mechanized excavation face; Mixed ventilation; Cutting dust; Diesel exhaust particles; Numerical simulation; The trackless rubber wheel car


### Z. Fallahnejad, Gh. Bakeri, A.F. Ismail. *Functionalized halloysite nanotubes incorporated thin film nanocomposite nanofiltration membrane for treatment of wastewaters containing metal ions*. Pages 334-351.


The high concentrations of heavy metal ions in industrial effluents are one of the most challenging wastewaters to deal with. In this study and in order to change the inner diameter of the halloysite nanotubes (HNT), their internal surface was coated by different polymers (polydopamine, polyaniline and polystyrene) and then, the modified nanotubes were incorporated in the polyamide thin film NF membrane for the treatment of metal ions solutions. Fourier Transform Infrared Spectroscopy (FTIR), X-ray diffraction (XRD) and Brunauer-Emmett-Teller (BET) studies indicated that the internal coating was successful. Furthermore, the neat and modified nanofiltration (NF) membranes were characterized in terms of morphology, contact angle, water flux and metal ion rejection. The modified membranes displayed lower contact angle values (29.4% reduction) that can be linked to the hydrophilic groups in the structure of the coated polymers and the

smoother surface of the thin film nanocomposite (TFN) membrane. In addition, the permeation fluxes of the modified membranes were improved significantly (33.4% improvement) without any major reduction in their ion rejection; that shows HNTs act as the channels to transfer water through the membrane structure while the coating of the inner surface of HNT reduces the size of the channel and makes more repulsion and steric hindrance for the ion to pass through the nanotubes. Among the fabricated membranes, the NF membrane with 0.05 wt% polystyrene-coated HNT showed the lowest contact angle (55.30o) and the highest water permeation flux (27.51 L m-2 hr-1), compared to the neat TFC membrane (15.26 L m-2 hr-1) and the NF membrane with 0.05 wt% unmodified HNT (20.62 L m-2 hr-1).

- **Keywords:** Thin film nanocomposite (TFN) membrane; Nanofiltration; Internal coating; Ion rejection; Halloysite nanotube (HNT)

### Wenli Feng, Yongfang Zhang, Liangliang Huang, Yunlin Li, Shuge Wang, Yi Zheng, Lei Shi, Ke Xu. *Source apportionment of environmentally persistent free radicals (EPFRs) and heavy metals in size fractions of urban arterial road dust*. Pages 352-361.

The partitioning of pollutants in the size-fractions of road dust particles is extremely important to their migration and bioavailability in the air environment. Herein, the pollution characteristics and sources of heavy metals (As, Cd, Cu, Cr, Pb, Zn, Co, Mn, Ni) and environmentally persistent free radicals (EPFRs) are investigated in 64 samples of mixed particle-size road dust in four size fractions (>250 μm, 150–250 μm, 75–150 μm,<75 μm). The samples were collected from urban arterial roads of three cities in the core of Central Plains Urban Agglomeration. The results indicate that 67.70% of the road dust (by mass) consist of the<75 μm particles size fraction, and that the highest levels of EPFRs and heavy metals are concentrated in the<150 μm and< 75 μm size fractions. In addition, Cd exhibits extremely high average enrichment factors (EFs) of 51.84 in the 75–150 μm fraction and 64.80 in the<75 μm fraction. Further analysis reveals a remarkable correlation between EPFR concentration and the concentrations Zn and Cr in the road dust. An application of principal component analysis (PCA) and positive matrix factorization (PMF) to the regional investigation and the layout of functional zones demonstrates that Cr, Pb, Zn and EPFRs are mainly derived from traffic emissions, and account for 51.45–77.86% of the fine particle fraction (<150 μm). Meanwhile, industrial activities are identified as the primary source of Cd and Cu, accounting for 63.07–76.22% of the<150 μm particle size fraction. These findings suggest a potential risk of EPFRs and heavy metals in fine particulate matter, and provide a new insight into the potential sources and health risks of EPFRs in road dust. Therefore, further studies are needed in order to explore the EPFRs in fine particulate particles and to assess their effects upon human health.

- **Keywords:** Road dust; Heavy metals; EPFRs; Source apportionment; PMF

### Qing Zhang, Dong Liu, Minjie Wang, Yixin Shu, Hailun Xu, Haiyan Chen. *Characteristics and evaluation index of pulse-jet dust cleaning of filter cartridge*. Pages 362-374.

In this study, we investigated the influence of tubular nozzle and upper opening diffuser on the performance of pulse-jet dust cleaning of filter cartridges through experimental tests. The optimal tubular nozzle injection distance was 200 mm, the sidewall pressure increased along the height of the filter cartridge, and the pressure at the lower part of the filter cartridge was much higher than that at the upper part. However, under the upper open diffuser, the uniformity of the pressure distribution along the height of the cartridge was effectively improved. Combined with the entropy weight method and considering the peak pressure and pressure uniformity, the integrated pressure was

proposed as a comprehensive index to evaluate the dust cleaning effect on filter cartridges. this result was verified using data from the literature , and can be used to evaluate the dust cleaning effect of filter cartridges.


- **Keywords:** Pulse-jet cleaning; Nozzle; Filter cartridge; Integrated pressure; Evaluation index


**Andres Gonzalez-Cortes, Damien Burlet-Vienney, Yuvin Chinniah, Abdallah Ben Mosbah, Ali Bahloul, Capucine Ouellet. *Inherently Safer Design (ISD) solutions in confined spaces: Experts' practical feedback in Quebec, Canada*. Pages 375-389.**


This paper aims to present solutions based on inherently safer design (ISD) principles to reduce the risks related to interventions in confined spaces and discuss their general applicability in a design situation or installations retrofit by exploring the client-designer relationship. A literature review on ISD solutions for confined spaces was followed by semi-structured interviews with 15 experts on confined space risk management in Quebec, Canada. The solutions based on the literature were confronted with experts' knowledge on the real-life conditions in confined space interventions. Our findings suggest that considering the entire confined space's life cycle in design is still very marginal (e.g., questioning the necessity to enter). As designers tend to replicate non intrinsically safe designs (e.g., inadequate entrances dimensions), end-users will then require retrofitting the structures over time, which usually costs more in the long term than implementing ISD solutions earlier. The notion of declassification of the confined space to eliminate confined spaces can give a false sense of safety. Its contribution to accident prevention depends on how end-users reduce inherent or task-induced risks as low as reasonably practicable. This paper categorized declassification into three types: total elimination, hazard-oriented declassification, and organizational declassification. Since the implementation guidelines of these risk reduction strategies are absent in the literature, this paper provides a risk reduction model that shows how end-users can identify application phases, declassify a confined space, and manage residual risks at the design phase in real-life environments.



- **Keywords:** Confined space; Declassification; Risk reduction; Inherently Safer Design; Accident prevention, Occupational health and safety


**Jianxin Zhang, Xiao Zheng, Yapei Cao, Zhigang Wang, Sibudjing Kawi, Xiaoyao Tan. *Tetraethylenepentamine-grafted polyacrylonitrile-poly(methyl methacrylate) hollow fibers for low concentration CO2 capture at ambient temperature*. Pages 390-396.**


In this work, a new type of solid amine sorbent was developed for low concentration CO2 capture at ambient temperature. Polyacrylonitrile(PAN)-poly(methyl methacrylate)(PMMA) porous hollow fibers were firstly prepared by a wet-spinning process. Tetraethylenepentamine(TEPA) was then grafted onto the porous structure of the hollow fibers. The amine modified hollow fibers denoted as TEPA@PAN-PMMA were characterized by the Fourier transform infrared spectroscopy (FT-IR), thermo-gravimetric analysis(TGA), Brunauer-Emmett-Teller(BET), and scanning electron microscopy(SEM) methods. Performance of the TEPA@PAN-PMMA for CO2 capture was evaluated by passing a 0.3% CO2-N2 gas mixture through the porous matrix of the hollow fibers at ambient temperature. The highest CO2 adsorption capacity reached up to 1.50 mmol g−1 for dry feed, and 3.00 mmol g−1 for wet feed, respectively. Cyclic CO2 adsorption-desorption test indicated that the TEPA@PAN-PMMA sorbents are stable and regenerable.

- **Keywords:** CO2 capture; Solid amine sorbent; Hollow fiber; Polyacrylonitrile(PAN); Poly(methyl methacrylate(PMMA)

**Yongming Han, Guangliang Song, Fenfen Liu, Zhiqiang Geng, Bo Ma, Wei Xu. *Fault monitoring using novel adaptive kernel principal component analysis integrating grey relational analysis*. Pages 397-410.**

The kernel principal component analysis (KPCA) is widely used as a fault monitoring tool for complex nonlinear chemical processes in recent years. The cumulative contribution rate that extracts the kernel principal is usually obtained relied on a fixed model, which cannot be employed for time-varying chemical processes. Hence, a novel adaptive kernel principal component analysis (AKPCA) integrating grey relational analysis (GRA) (AKPCA-GRA) is proposed to dynamically monitor the fault occurrence. A moving window integrating the threshold method is used to adaptively extract the kernel principal for chemical processes. Then the corresponding T2 and Q statistics calculated by the selected kernel principal based on the AKPCA decides whether the fault has occurred. Moreover, the GRA method is used to analyze and calculate the correlation coefficient of abnormal features obtained based on the APKCA method, which provides the operational guidance for the nonlinear chemical process to find out the variable causing the fault. Finally, the proposed method is verified using the Tennessee Eastman (TE) process. The case results demonstrate that the proposed method outperforms the KPCA, the KPCA based on the threshold and the moving window principal component analysis, the support vector machine (SVM) and the Logistic Regression (LR) in terms of the missed alarm rate (MAR) and the false alarm rate (FAR), which can effectively analyze the variables causing the fault.

- **Keywords:** Adaptive kernel principal component analysis; Threshold method; Moving window; Fault monitoring; Grey relational analysis; Chemical process

**Fu-Xin Dong, Liu Yan, Shi-Ting Huang, Jing-Yi Liang, Wen-Xuan Zhang, Xiao-Wen Yao, Xie Chen, Wei Qian, Peng-Ran Guo, Ling-Jun Kong, Wei Chu, Zeng-Hui Diao. *Removal of antibiotics sulfadiazine by a biochar based material activated persulfate oxidation system: Performance, products and mechanism*. Pages 411-419.**

Nowadays, the harm of antibiotics residues in environments to human health and ecological safety has been causing more and more attention. In this paper, a biochar based iron material (MBC) was used to activate persulfate (PS) for the removal of sulfadiazine (SDZ) from aqueous solution. Experiment results indicate that the degradation and mineralization of SDZ by MBC/PS system reached 91.79% and 60% within 60 min under the optimal reaction conditions, respectively. MBC/PS system exhibited a better performance on SDZ removal compared with MBC/H2O2 system. The addition of Cu2+ ion could enhance the degradation of SDZ by MBC/PS system. PO43-, Cl- and SO42- had a certain degree of inhibitory effect on the SDZ degradation. Both radicals and non-radical species such as SO4•-, •OH and 1O2 participated in the degradation reaction of SDZ by MBC/PS system, but •OH was the main radical species responsible for SDZ degradation. The liquid chromatograph-mass spectrometer (LC-MS) technique was used to identify the intermediate products of SDZ, and it was proposed that the degradation of SDZ might be achieved through hydrolyzation, hydroxylation, deamination and amino-oxidization processes. A possible reaction mechanism involving a synergistic effect between PS homogeneous and heterogeneous activation processes as well as both radicals and non-radicals reactions was finally proposed.

- **Keywords:** Sulfadiazine; Biochar; Iron material; Persulfate; Antibiotics degradation

**Wen-Hsing Chen, Yun-Ting Luo, Jih-Gaw Lin, Yu-Tzu Huang. *Facultative-like anaerobic packed bed reactor treating low strength wastewater: microbial community and energy balance appraisements*. Pages 420-428.**

This study explored the microbial community and the energy requirement of an anaerobic packed bed reactor (APBR) treating a low-strength synthetic wastewater (200 mg COD/L). The APBR was run with different hydraulic retention times (HRTs) and temperatures. Results show that the COD removal decreased from 89 to 46% when the HRTs and the temperature were both gradually reduced to 1 h and 20°C. Meanwhile, the methane yield decreased from 0.386 to 0.232 g COD/g TCODconsumed with the decreasing temperature from 35 to 20°C at 1-h HRT. This low methane production was associated with a low relative abundance of 0.575–0.628% for the archaea group in genus level. Genus Methanosaeta with 0.307–0.388% relative abundance represented 53–62% of the archaea group whereas facultative Trichococcus with 7.3–11.3% relative abundance was dominant in the microbial consortia. Candidatus Moduliflexus found was the second largest microbial population with 4.2–6.1% relative abundance. This facultative environment was observed in the APBR, resulting in 18–37% COD unbalanced. The energy appraisement resolved that the total electrical energy required for the APBR was consistent at 4.192 × 10−3 kWh/m3 at 20–35°C to yield the net energy ratio of 5.97–15.29. The facultative-like APBR treated the low strength wastewater efficiently while the energy input was balanced by its self-produced methane energy.

- **Keywords:** Anaerobic filter; Facultative bacteria; Sewage; 16S metagenomic sequencing; Uncultured bacteria

**A.L. Ramírez-Ledesma, J.A. Juárez-Islas. *Modification of the remaining useful life equation for pipes and plate processing of offshore oil platforms*. Pages 429-442.**

Incorporation of an adequate maintenance program related to the ageing of industrial facilities occurring in offshore oil platforms is vital to reduce costs and avoid catastrophic failures. In the present work, a set of components (i. e. pipes, plates, and elbows) were removed from offshore oil platforms from different processes with 20 years of uninterrupted operation. The component's characterization consisted of chemical composition, microstructure, and mechanical properties. A collection of results was made to evidence several indicators to keep track of crucial deviations of processing components. These indicators should be taken into account when actions must be taken to guarantee the mechanical integrity of the studied components. From 68 studied samples, 16 samples did not fulfill their chemical composition, 37 samples showed a banded microstructure, 36 samples did not fulfill their mechanical properties, and all of them showed the presence of non – metallic inclusions associated with a pitting corrosion mechanism. These results compilation allow for modification of the remaining useful life equation, RUL, (used to calculate the remaining useful life of a variety of asset types). Thus, the outcome of the modified equation indicates where and when it is necessary to remove components before its catastrophic failure.

- **Keywords:** Ageing; Offshore oil platforms; Degradation; Remaining useful life equation

**Hepeng Yin, Huaming Dai, Guangqian Liang. *Inhibition evaluation of magnesium hydroxide, aluminum hydroxide, and hydrotalcite on the flame propagation of coal dust*. Pages 443-457.**

Coal dust suspended in a syngas atmosphere may result in a dust explosion during the coal gasification process. A vertical tube with a high-speed camera and thermocouple was built to investigate the flame propagation characteristics of coal dust. Magnesium hydroxide (MH), aluminum hydroxide (ATH), and hydrotalcite (HT) were selected as the inhibitors to compare their inhibition effect. The results showed that the effects of the three inhibitors differed greatly. The addition of MH prolonged the flame propagation time, but its inhibition of flame temperature was the worst. The peak temperature and velocity of the flame after the addition of HT were the smallest compared to that after the addition of MH and ATH. Besides, the analysis of residues proved that the unburned coal dust was completely encapsulated by the high-temperature resistant oxides from HT so that the coal dust was most effectively protected, which showed the best heat absorption properties and the lowest decomposition temperature compared with that of MH and ATH.


- **Keywords:** Coal gasification; Coal dust deflagration; Hydrotalcite dust; Inhibition mechanism


**Xiaohang Zhang, Yanping Liu, Ming Wei, Jinlong Tan, Tingchao Yang, Xuwen He. *Influence of ballasted material properties in enhancing the separation of high concentration suspended solids in coal mining water*. Pages 458-465.**


With the continuous improvement and economic development of China's coal mining industry, research on the characteristics of wastewater discharge has gained attraction in recent years. Ballasted flocculation technology, has been widely used in recent years. However, its effect on the settling velocity of the flocs in wastewater has not been quantified. This study aimed to screen optimal reaction condition for ballasted flocculation and to derive the settling velocity of the ballasted flocs under these conditions. The results showed that, the size of the ballasted material had no significant effect on the turbidity and suspended solids removal rate; however, the settling time was effectively shortened, and the turbidity removal rate could reach more than 95% within 15 s. Owing to the optimization of the reaction conditions, 90% of the flocs sizes were distributed in the 80–200 μm range. Moreover, the difference between the theoretical and the measured value of the ballasted flocculation was small, indicating that the derived formula could effectively quantify the settling velocity of the ballasted flocs under optimal conditions. These findings may serve as a critical reference for the treatment of high-suspended solids in coal mining water and have significant potential for engineering application.



- **Keywords:** Ballasted flocculation; Fractal dimension; Settlement velocity; Stress analysis; Coal mining water


**Yue Yue, Wen-mei Gai, Yun-feng Deng. *Influence factors on the passenger evacuation capacity of cruise ships: Modeling and simulation of full-scale evacuation incorporating information dissemination*. Pages 466-483.**


The passenger evacuation capacity (PEC) of a cruise ship is a pivotal guarantee for quickly and safely evacuating all personnel on a damaged ship during an emergency. A general framework of the agent-based evacuation model is proposed in this study to simulate the entire process of cruise ship evacuation. The total evacuation time, duration of Level of Service (LOS) lower than E, effective flow rate of the escape route, density of the muster station, and usage rate of the lifeboat/life raft are used as the five evaluation indicators to quantify the PEC of cruise ships, thus providing a reference for the optimization analysis of evacuation procedures. With this framework, the PECs under different evacuation strategies of a cruise ship were evaluated in the context of ship

heeling to capsizing for the Yangtze Gold 1. Evaluation results show that the increase of heeling angle when the evacuation order is issued does not affect the perception time of the first 90% of evacuees, but significantly increases the total evacuation time after more than 20°. Moreover, the degree of regional congestion is affected by several factors, including the assignment of muster stations, evacuation in batches, the place of obtaining life jackets, the heeling angle, the difference of escape route flows, and other factors. The results of this study provide PECs under different strategies as references for specific accident scenarios and evacuation targets.


- **Keywords:** Evacuation model; Cruise ship; Information dissemination; Evacuation strategy; Passenger evacuation capability


**Hayder A. Alhameedi, Aso A. Hassan, Joseph D. Smith. *Towards a better air assisted flare design for low flow conditions: Analysis of radial slot and flow effects*. Pages 484-492.**


Numerical investigation of flow field characteristics of air injected through an inclined radial slot into a crossflowing stream has been studied for gas flaring applications. CFD is used to simulate turbulent mixing between the inclined slot jet and the crossflowing stream. The slot injection angle with respect to the crossflow, the slot jet velocity, and the slot height were varied in this study. Velocity profiles obtained from the simulations were compared to measured profiles. Simulation results showed that the centerline upflow axial velocities increased with decreasing injection angle and increasing slot height. Results also showed that decreasing injection angle increased the horizontal penetration of the jet flow into the crossflow stream.



- **Keywords:** Inclined slot jet; Radial velocity profile; Computational fluid dynamics (CFD); Air-assisted flare; Purge flow condition


**Shan Lyu, Shuhao Zhang, Xiaomei Huang, Shini Peng, Jun Li. *Investigation and modeling of the LPG tank truck accident in Wenling, China*. Pages 493-508.**


In this study, the liquefied petroleum gas (LPG) accident in Wenling, Zhejiang Province, China, on June 13, 2020, was analyzed and simulated. An LPG tank truck overturned and collided with the concrete guardrail; the subsequent explosion of the tank released 25.36 t LPG. Shortly afterward, the LPG tank was shot into the air, and the gas cloud ignited, thereby triggering a fire and vapor cloud explosion (VCE). This accident killed 20 people, injured 175 people, and caused significant property loss. The accident timeline was established based on multiple accident images, and the accident process was discussed in detail. The distribution of tank debris, evaporation and spreading of the LPG pool, dispersion of the LPG gas cloud, and VCE were simulated with the EFFECTS and ALOHA software. The images of the accident scene helped to determine and analyze the accident process. In the particular case in which a tank is shot into the air with a continuous two-phase jet, the actual flight distance of the tank is much greater than the prediction of the debris distribution model. The gas cloud distribution simulated with the SLAB model approximately corresponds to a major part of the severely damaged zone. In this accident, the TNO multi-energy method and ALOHA provide relatively consistent predictions with the actual building damage distribution when models use a specific confined explosive mass.



- **Keywords:** LPG release; BLEVE; Vapor cloud explosion (VCE); Accident investigation; Accident modeling


**Tongyuan Yang, Yang Xue, Xiaoming Liu, Zengqi Zhang. *Solidification/stabilization and separation/extraction treatments of***

***environmental hazardous components in electrolytic manganese residue: A review*. Pages 509-526.**

Electrolytic manganese residue (EMR), a by-product of the electrolytic manganese metal production process, contains several hazardous components such as ammonia nitrogen (NH3-N), soluble manganese, and heavy metals. In recent years, although a great number of treatment methods have been proposed, there is no mature and economical industrial process for treating EMR. Therefore, previous studies on separation/extraction (S/E) and solidification/stabilization (S/S) treatments of EMR are reviewed and are of great significance for further studies. The various treatment methods are summarized and evaluated, and the existing problems or prospects are given. The use of external field enhancement methods and appropriate auxiliary leaching agents in the S/E process can effectively improve the leaching efficiency. In the S/S treatment, it is found that the synergism of multiple solid wastes can increase the waste treatment capacity, which has significant environmental benefits and even can realize resource utilization. The research on manganese treatment has been found to have achieved remarkable results, but the problem of ammonia nitrogen in EMR still cannot be ignored and future research still has challenges. Further, based on the existing problems with harmless treatments of EMR, some suggestions are provided and the remaining challenges for future research are identified.

- **Keywords:** Electrolytic manganese residue; Environmental hazardous components; Separation/extraction; Solidification/stabilization; Mechanism of action; Heavy metal

**Jincheng Lu, Qiongfang Zhuo, Xiuwen Ren, Yongfu Qiu, Yanliang Li, Zhongying Chen, Kaifeng Huang. *Treatment of wastewater from adhesive-producing industries by electrocoagulation and electrochemical oxidation*. Pages 527-536.**

Adhesive wastewater from adhesive-producing industries is a kind of refractory organic wastewater containing high chemical oxygen demand (COD) and ammonia nitrogen. In this study, the electrocoagulation and electrochemical technology were in series attempted to treat adhesive wastewater from adhesive-producing industries. The effects of operating parameters such as current density and initial pH were investigated to determine the optimum electrocoagulation parameters. The removals of COD and ammonia nitrogen achieved 81.62%, and 50.92%, respectively, under the optimum electrocoagulation conditions (current density of 5 mA/cm2, pH 3, 2 g/L Na2SO4 supporting electrolyte solution, 60 min of electrocoagulation). The effluent of electrocoagulation was subsequently treated by electrochemical oxidation. The effects of operating parameters, such as current density, initial pH, and supporting electrolyte, on the degradation of COD and ammonia nitrogen were investigated. The COD and ammonia nitrogen removal ratios were both as high as nearly 100% after electrolysis of 120 min (current density of 35 mA/cm2, pH 8.4, 2 g/L NaCl supporting electrolyte solution). The results of excitation-emission-matrix (EEM) revealed the changes of different dissolved organic matter after electrocoagulation and electrochemical oxidation treatment. The experimental results proved that the electrocoagulation combined with electrochemical oxidation methods are the potential technologies for treatment of adhesive wastewater.

- **Keywords:** Adhesive wastewater; Electrocoagulation; Electrochemical oxidation; Dissolved organic matter; COD Removal; Ammonia nitrogen removal

**Victor Rezende Moreira, Yuri Abner Rocha Lebron, Carolina Fonseca Couto, Andreza Maia, Wagner Guadagnin Moravia, Miriam Cristina Santos Amaral. *Process development for textile wastewater treatment towards***

***zero liquid discharge: Integrating membrane separation process and advanced oxidation techniques*. Pages 537-546.**

A treatment process based on microfiltration followed by nanofiltration (MF-NF) is proposed for textile wastewater treatment. The NF concentrate is further treated by UV/H2O2, Fenton, and photo-Fenton processes. Results showed that the dye was efficiently retained by the MF membrane (>99.1%), which allowed its reuse. The MF-NF was able to reject 92% of the chemical oxygen demand (COD) and>98.5% of color. When the NF concentrate was treated by UV/H2O2, it was achieved a maximum COD removal of 63% in the condition C:H2O2 1:3 (molar ratio of COD and hydrogen peroxide) and pH 3. The Fenton process, optimized through response surface methodology, achieved 84.7% of COD removal, which increased when combined with UV irradiation (92.2%). An analysis of the NF permeate physicochemical quality and its treated concentrate suggested that it can be reused in the textile industry for different purposes as yarn washing-off and equipment's washdown. The operating cost for MF-NF corresponded to 0.240 US$/m3 and, including the cost of NF concentrate treatment by photo-Fenton, 0.517 US$/m3, lower than currently practiced by the water distribution company. The system proposed for water reuse and NF concentrate treatment was able to increase the water recovery and decrease the environmental impacts that could be caused by the NF concentrate disposal.

- **Keywords:** Integrated treatment process; Dye recovery; Membrane technology; Advanced oxidation processes; Water reclamation