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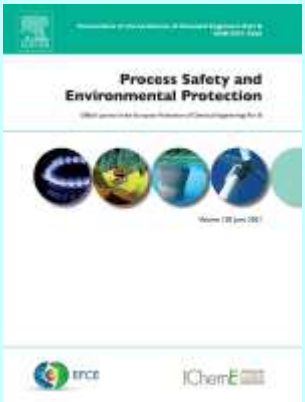

Yonghao Zhou, Yanchao Li, Haipeng Jiang, Kai Zhang, Xiangfeng Chen, Lei Huang, Wei Gao. *Investigations on unconfined large-scale methane explosion with the effects of scale and obstacles*. Pages 1-10.

The strong pressure wave in gas explosion accident could cause great casualties and property loss, which has become the main threat to safety of chemical process and further popularization of clean energy. In this research, unconfined explosion experiments under different methane concentrations at 27 m3 scale were performed with internal and external obstacles. The results showed that the flame buoyant effect was more obvious for the rich-fuel flame due to the excess methane accumulation. The reflection of the pressure wave could cause higher overpressure near the ground and the external obstacle enhanced the overpressure in the neighborhood. For 27 m3 scale explosion, the critical flame radius for the flame acceleration was larger than 1 m3 scale, because of the longer travelling distance for the reflection wave from the bottom. In addition, the acceleration exponent rose to 1.5 due to the full development of the hydrodynamic instability. The flame radius for peak overpressure, RM, was found to be at a certain distance from the outer obstacle bar center, which was 1.8 for Nb = 6, 1.35 for Nb = 4 and 0.9 for Nb = 2. The predicted results of peak overpressure agreed well with the experimental results, which extended the prediction model to the larger scale.

- **Keywords:** Unconfined methane explosion; Obstacle disturbance; Scale effect; Overpressure prediction

Sirajum Monira, Muhammed A. Bhuiyan, Nawshad Haque, Biplob Kumar Pramanik. *Assess the performance of chemical coagulation process for microplastics removal from stormwater*. Pages 11-16.

Microplastic (MP) is considered as one of the emerging pollutants in marine environments. Because of low density and small particle size (<5 mm), MPs are easily discharged into open waterways by stormwater runoff. Therefore, the aim of this study was to investigate the effect of coagulation process for the removal of different types of MPs such as low-density polyethylene (LDPE), high-density polyethylene (HDPE) and polypropylene (PP) from synthetic stormwater. The effect of different types of a

coagulant such as alum and polyacrylamide (PAM), dosages of coagulants, solution pH and weathering conditions was investigated for the removal of MPs. Results found that a combination of alum and PAM performed better than standalone coagulant for MPs removal. The removal of all three types of MPs was high at low pH (3–5). It is also found that the removal efficiency of LDPE, HDPE and PP was 92 %, 84 % and 96 %, respectively under the weathering conditions. The mechanisms for MP removal were charge neutralization and hydrophobic interaction between MP and coagulant flocs. Overall, this study has confirmed that the coagulation process was very effective for removing MP particles under weathering conditions.

- **Keywords:** Coagulation; Humic substances; Microplastics; Marine environments; Stormwater

Hüseyin Yağlı, Yıldız Koç, Özkan Köse, Ali Koç, Recep Yumrutaş. *Optimisation of simple and regenerative organic Rankine cycles using jacket water of an internal combustion engine fuelled with biogas produced from agricultural waste*. Pages 17-31.

Internal combustion engines have a very important place in biogas production facilities to convert biogas energy to electricity. Unfortunately, although intense studies on improving internal combustion engine efficiencies by operational optimisation methods, serious progress is not achieved yet. However, there are many ways to improve the performance of these engines apart from structural optimisation methods. One of the most important ways is to utilize by integrating jacket water used to cool the biogas fuelled internal combustion engines into the new generation low-temperature heat recovery systems like organic Rankine cycles. In the present study, simple and regenerative organic Rankine cycles were optimised to improve the overall performance of an biogas fuelled internal combustion engine by using the jacket water which is released into the atmosphere after cooling the engine. Also, the energy, exergy and environmental aspect of these systems are evaluated. Finally, exergoeconomic analysis for both systems are conducted, and then payback periods of both systems are determined. As a result of the study, the maximum net power, thermal and exergy efficiencies of the simple organic Rankine cycle was calculated as 42.14 kW, 11.47 % and 63.27 % respectively, while the maximum net power, thermal and exergy efficiencies of the regenerative organic Rankine cycle are found as 45.3 kW, 12.34 % and 68.02 %. In addition, it is observed that the maximum power production obtained from the regenerative organic Rankine cycle corresponded to nearly 630 kg CO2/h emission reduction. The best payback period value is also calculated as 7.37 years in the simple organic Rankine cycle.

- **Keywords:** Biogas engine; Organic Rankine cycle; Biogas; Jacket water; Agricultural organic waste; Environment; Exergoeconomic

Xiaoyan Liu, Xintong Chen, Xinying Zhang, Hao Guo, Changsong Zhang, Xueke Zang, Beibei Li. *Quantifying the influence of soil factors on the migration of chromium (VI)*. Pages 32-40.

Identification of the factors controlling the migration of hexavalent chromium (Cr (VI)) in soil can provide valuable information for pollution control and risk assessment. In this study, we assessed the processes of transportation and migration of Cr (VI) in soil by batch and column experiments. Breakthrough curves were used to examine the mobility of Cr (VI) in soil columns. Most of them could be described by a typical S-shaped curve. The Yoon–Nelson model and Thomas model were applied to predict the behavior of Cr (VI) in soil and obtained parameters to characterize the rate and capacity of adsorption. It was observed that all obtained parameters changed along with soil properties. Moreover, stepwise multiple regression and grey correlation analysis were used to determine the main control factors by evaluating the relationship between soil properties

and dynamic or static parameters. The results showed Fe oxide content was the key factor no matter in static or dynamic adsorption while soil texture had a great influence on the transportation of Cr (VI) in soil columns. Also, in the actual situation, the external input condition should not be ignored. Our research provides meaningful information for authorities to develop better soil management and remediation strategies.

- **Keywords:** Chromium adsorption; Breakthrough curve; Regression model; Grey correlation analysis

Xiayuan Feng, Yiyang Dai, Xu Ji, Li Zhou, Yagu Dang. *Application of natural language processing in HAZOP reports*. Pages 41-48.

Accidents in chemical production usually result in fatal injuries, economic losses, and negative social impacts. To ensure personnel security in such cases, previous research has often used digital data, such as physical signals. However, the valuable textual information contained in chemical security texts, such as expert knowledge, has not yet been explored. Therefore, there is an increasing demand to mine useful information from these unstructured data. In this study, natural language processing (NLP) was applied to the hazard and operability (HAZOP) analysis reports. The classification model was trained to learn the classification of consequence severity levels in high-quality HAZOP analysis reports, which will not only ensure the consistency of the analysis results, but also help smaller chemical plants perform security analysis. In the classification model, we introduced Bidirectional Encoder Representation from Transformers (BERT), which, for word embedding, which is a powerful NLP pre-training model and significantly improved the effectiveness of the model. Through these application scenarios, the feasibility and possibility of applying NLP in chemical security text have been confirmed to a certain extent. In addition to digital data, future security managers will be able to monitor chemical production using natural language.

- **Keywords:** NLP; Chemical process safety; HAZOP reports; Text mining; BERT

Asim Ali Yaqoob, Mohamad Nasir Mohamad Ibrahim, Susana Rodríguez-Couto, Akil Ahmad. *Preparation, characterization, and application of modified carbonized lignin as an anode for sustainable microbial fuel cell*. Pages 49-60.

Microbial fuel cell (MFC) is the most prominent bioelectrochemical approach in electricity generation while metal removal is its secondary application. However, ongoing challenges including low electron transfer rates and unstable biofilm formation on the anode surface need to be addressed. As an attempt to overcome such drawbacks, in the present study, the anode was prepared from graphene oxide (Lg-GO) obtained from lignin and subsequently modified with a metal oxide (i.e., TiO2). Thus, the plain Lg-GO and Lg-GO/TiO2 delivered 57.01 mA/m2 and 70.17 mA/m2 of current density along with 85 % and 90 % of Pb (II) ions removal from synthetic wastewater, respectively within the 90-day operation of MFC. The recorded maximum power density at the Lg-GO anode was 0.44 mW/m2, while the maximum PD at the Lg-GO/TiO2 anode was 0.78 mW/m2. The prepared anodes were characterized, and the operational conditions were optimized to validate their performances. The results showed that the optimum performance of the anode was in normal environmental conditions (e.g., pH 7, room temperature). In conclusion, the obtained results indicated that the prepared electrodes (i.e., Lg-GO and Lg-GO/TiO2) are suitable for energy generation and metal removal via MFC.

- **Keywords:** Microbial fuel cell; Energy generation; Wastewater treatment; Anode fabrication; Lignin

Zhenjuan Gao, Jianchun Miao, Jingfeng Zhao, Mehdi Mesri. *Comprehensive economic analysis and multi-objective optimization of an integrated gasification power generation cycle*. Pages 61-79.

A novel power generation plant was devised based on the biomass integrated fired combined cycle as the central unit and supercritical CO2 cycle, regenerative organic Rankine cycle, and steam Rankine cycle as the waste heat recovery subsystems. Exergoeconomic and economic criteria were defined to evaluate the feasibility of the system for investment and construction. Thus, net present value, payback period, and sum unit cost of products were considered as the system's evaluation criteria from the economic viewpoint. The system was firstly analyzed by developing a precise model in the Engineering Equation Solver. Then, optimal conditions were obtained by coupling the outputs of modeling procedure with artificial neural network, multi-objective particle swarm optimization, and the technique for order of preference by similarity to ideal solution (TOPSIS) approaches. It was concluded that the system has an exergy efficiency of 42.7 % with a power generation capacity of 7.768MW, a total cost rate of 34.79 $/GJ, and a total profit and payback period of 23.3 $M and 5.7 years. For the optimization results in the ε-NPV-SUCP scenario, the optimum values of 58.99 %, 30.6 $M, 35.61 $/GJ were obtained for exergy efficiency, NPV, and SUCP, respectively.

- **Keywords:** Power generation cycle; Biomass integrated combined cycle; Economic analysis; Artificial neural network; Multi-objective optimization

Douglas Thiago S. Alves, Gilson Brito Alves Lima. *Establishing an onshore pipeline incident database to support operational risk management in Brazil - Part 2: Bowtie proposition and statistics of failure*. Pages 80-97.

In part 1, which is complementary to this article, an appropriate data collection architecture was proposed in order to support the establishment of an onshore pipeline incident database in Brazil. Reflecting the current context of pipeline industry in this country, this structure was built based on the state of art regarding several international databases followed by an interdisciplinary survey submitted to pipeline experts from different areas of specialization. According to their favorability, a criteria was applied in order to select the collection parameters that, finally, compose the proposed architecture. In this second paper (part 2), a bowtie diagram was elaborated inspired on the results obtained in part 1 in order to support the management of onshore pipelines operational risks. In addition to defining causes and consequences, prevention and mitigation barriers along with respective leading and lagging indicators were elucidated based on the literature allowing pipeline operators to monitor the status of these controls over time and contributing to the improvement of their risk management systems. Additionally, failure statistics similar to those presented by international benchmark reports were developed through historical failure data obtained from a Brazilian pipeline operator. Among other metrics, it is reproduced the behavior of failure rates along the period in analysis (from 1978 to 2008), as well as distributions of incidents by categories of causes and exposure (extension) evolution of the pipeline network considered. In sequence, a comparison between Brazilian and international benchmarks failure frequencies is performed. Finally, illegal tapping statistics from 2016 to 2020 are also addressed, indicating some prevention and mitigation measures that were implemented in this period in order to better manage operational risks associated with pipeline theft.

- **Keywords:** Pipeline incident database; Pipeline process safety; Bowtie diagram; Pipeline failure frequencies; Operational risk management; Pipeline theft

Richard Kuracina, Zuzana Szabová, Marián Škvarka. *Study into parameters of the dust explosion ignited by an improvised explosion device filled with organic peroxide*. Pages 98-107.

Dust explosion poses a significant hazard in industry. An explosion of dispersed dust can be ignited by an improvised explosive device. The article deals with the study of explosion parameters of representative samples of dispersed dust ignited by an improvised explosive device. Hexamethylene triperoxide diamine was used as an igniter. Lycopodium clavatum spores were used as a standard sample. Furthermore, dust samples were selected from those types of operations that may be endangered if an improvised explosive device is used as an igniter. Wheat flour and beech wood dust were selected as representative samples. The achieved parameters of explosion pressure and explosion constant Kst were on average by 5–15% lower than the parameters achieved when using a commercial igniter. The Pmax value and the inflection point of the explosion record were reached 7–12 ms earlier than those achieved with a commercially available igniter. The findings may be relevant in the design of explosion prevention devices. New types of explosion prevention devices can be designed to reduce the risk of explosion of dispersed combustible dust caused by improvised explosive devices, e.g. in a case of terrorist attack on the objects with the occurrence of dust clouds.

- **Keywords:** Flammable dust; Dust explosion; Hexamethylene triperoxide diamine; Lycopodium clavatum spores

Siti Shilatul Najwa Sharuddin, Siti Rozaimah Sheikh Abdullah, Hassimi Abu Hasan, Ahmad Razi Othman, Nur 'Izzati Ismail. *Potential bifunctional rhizobacteria from crude oil sludge for hydrocarbon degradation and biosurfactant production*. Pages 108-121.

Biosurfactant produced by rhizobacteria has the potential to enhance the degradation of hydrocarbons, leading to more efficient phytoremediation. The aim of this work was to search for bifunctional hydrocarbon-degrading and biosurfactant-producing rhizobacteria. Isolation of bacteria was conducted from three sources (A: rhizosphere of Scirpus grossus planted in garden soils and B: rhizosphere of S. grossus planted in crude oil sludge and C: crude oil sludge) prior to degradation test. Seven isolated rhizobacteria from source B (coded as B1–B7) were screened for a hydrocarbon degradation test with an initial total petroleum hydrocarbon content of 56.13 mg/g. Similar isolated rhizobacteria were also found in source A and C. The best three isolates (B1, B3 and B6) and mixed culture of them, significantly degraded hydrocarbon with 16.2%, 8.4%, 39.7% and 34.8% removals, respectively. Subsequently, the three pure rhizobacteria and their mixture (B1 + B3 + B6) were screened for biosurfactant production through tests of oil displacement, drop collapse, emulsification and surface tension. All the pure rhizobacteria and mixed culture had given positive response for all the tests. The presence of biosurfactant produced by rhizobacteria was confirmed by SEM images in which the formation of exopolymers interconnecting individual cells into a complex network of mass was formed due to biosurfactant extraction from bacteria cell. Thus, the three isolated rhizobacteria (B1, B3, and B6), later identified as Bacillus sp. strain SB1, Bacillus sp. strain SB3 and Lysinibacillus sp. strain SB6, respectively, and their mixed culture can simultaneously biodegrade hydrocarbon and produce biosurfactant to enhance the degradation process.

- **Keywords:** Biosurfactant; Hydrocarbons; Rhizobacteria; Biodegradation; Surface tension; Bioremediation

Dandan Wang, Changtai Song, Bingliang Zhang, Jingwen Chen, Ailan Luo, Xiaosan Wang, Shengde Wu, Yuxuan Ye. *Deciphering dissolved*

***organic matter from freshwater aquaculture ponds in Eastern China based on optical and molecular signatures*. Pages 122-130.**

Aquaculture makes great contribution to global food production. The aquaculture capture scale of China was far ahead of other countries in the world. Despite the potential role of dissolved organic matter (DOM) to affect fish growth and ecological cycle, the characterization of DOM in aquaculture industry was poorly understood. In this study, fluorescence excitation-emission matrix (EEM) spectroscopy and Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS) were conducted to decipher the optical and molecular signatures of DOM in freshwater aquaculture ponds in Eastern China. The EEM dataset was decomposed by parallel factor analysis (PARAFAC). Three main components including humic/fulvic acid-like (C1 and C3), tryptophan-like (C2) and tyrosine-like substances (C3) were obtained. FT-ICR-MS identified DOM composition at molecular level. In terms of formula classes, the dominant CHO species were followed by CHON and CHOS groups. According to compound classification criteria, the key components of lignins, tannins, proteins and lipids illustrated the primary source from terrestrial sediment, feeding doses and stocked creatures, implying the great influence by the land-based aquaculture ponds. Typical spectral indexes such as humification index (HIX), biological index (BIX) and fluorescence index (FI) consistently reflected the lower humification degree of DOM and greater contribution from protein-like sources. Furthermore, to utilize readily available spectral indexes to predict the time-consuming molecular properties, redundancy analysis and the pairwise correlation analysis was carried out to prove that two spectral indexes (E2:E3 and BIX) were negatively associated with four molecular formula derived parameters (O/Cwa, AImodwa, DBEwa and NOSCwa). The findings expanded our understanding of aquaculture DOM evolved in environmental chemistry.

- **Keywords:** Dissolved organic matter; Aquaculture; EEM; FT-ICR-MS; Molecular composition; Redundancy analysis

Mengchu Song, Morten Lind, Jun Yang, Akio Gofuku. *Integrative decision support for accident emergency response by combining MFM and Go-Flow.* Pages 131-144.

Emergency response planning associated with written procedures play a key role in the process safety to ensure that accident can be properly managed. Although the extensive use of digital techniques have significantly reduced the accident risk by early warnings and operation guidance, the Fukushima nuclear disaster reminds us that the unexpected events may still exceed existing system capability to indicate appropriate responding measures. A novel digitalized approach is hence required for planning decision support. This article presents a joint utilizing of two modeling and analysis methodologies, which are complementary to each other to provide comprehensive insights for decision-making in the accident emergency response. Multilevel Flow Modeling (MFM) is applied to develop an intelligent reasoning system, which can harness plant's qualitative functional knowledge to search available equipments and corresponding action sequences potentially being able to manage the accident. Go-Flow is a success-oriented reliability analysis method specially suitable for quantitative risk assessment in the situations involving configuration changes. The underlying configuration of each MFM-driven emergency response measure will update the understanding of goal achievement and modify the Go-Flow chart, by which plan's effectiveness of risk reduction can be evaluated. Moreover, Go-Flow is also used to conduct the risk matrix assessment for identifying critical components, which can provide a reference for effective assignment of resources in the long-term accident management. This work is expected to strengthen operator's ability of emergency response planning from perspective of both measure development and optimization. An accident scenario similar to what occurred in the Fukushima Daiichi nuclear power plant has been used to demonstrate the application of the propose approach.

- **Keywords:** Emergency response planning; Accident management; Decision support system; Multilevel Flow Modeling; Risk-informed decision-making; Success-oriented Go-Flow

Byoungjik Park, Yangkyun Kim, Shinwon Paik, Chankyu Kang. *Numerical and experimental analysis of jet release and jet flame length for qualitative risk analysis at hydrogen refueling station*. Pages 145-154.

The advent of eco-friendly hydrogen vehicles has prompted attempts to increase the installation of hydrogen refueling stations in urban areas; however, sufficient safety measures have yet to be established. Gas plume dispersion, jet flame, and heat flux were investigated using HyRAM software by considering accidents at hydrogen refueling stations in reports published by Sandia National Laboratories. Hydrogen release and jet flame length were measured using the Schlieren imaging system and a thermal imaging camera. The HyRAM simulation analysis results were more conservative than the experimental results. These showed that the pressure and leak diameter greatly influenced the safety of hydrogen facilities. Individual and societal risks were analyzed through RISKCURVES, and the risks were found to be highest in the sidewalk and dispenser. An F-N (Frequency- Number of fatalities) curve to verify the risk of installing a hydrogen refueling station in urban areas was derived, and the safety distance from residents was proposed.

- **Keywords:** Hydrogen refueling stations; HyRAM; Schlieren imaging system; RISKCURVES; F-N curve

Wei Han, Wenbiao Jin, Ze Li, Yubin Wei, Zhongqi He, Chuan Chen, Changlei Qin, Yidi Chen, Renjie Tu, Xu Zhou. *Cultivation of microalgae for lipid production using municipal wastewater*. Pages 155-165.

The shortage of energy and the aggravation of eutrophication are two major problems in China. The use of municipal wastewater to cultivate lipid-producing microalgae for the production of biodiesel not only reduces the production cost of biodiesel and alleviates energy shortage, but also mitigates eutrophication and protects the water environment. This study explored the effects of light, pH, and nutrients on the growth and lipid production of Scenedesmus obliquus, as well as the lipid production and pollutant removal capabilities of algae during microalgae cultivation in municipal wastewater at different treatment stages. The optimal conditions for the growth and lipid production of S. obliquus were determined as light intensity of 14,500 lx, total nitrogen (TN) content of 97 mg L−1, total phosphorus (TP) content of 11 mg L−1, and CO2 content of 9.8%. Under these optimal conditions, the lipid yield from microalgae was 0.367 g L−1, which was superior to other optimisation results in the literature. The total lipid yields of S. obliquus cultivated in the wastewater from the primary and secondary settling tanks were 0.38 g L−1 and 0.33 g L−1, respectively. The TN and TP removal rates were 99.8% and 83.1% from the wastewater of the primary settling tank, and 98.9% and 97.6% from the wastewater of the secondary settling tank, respectively. In addition, fluctuations in the quality of raw wastewater may lead to fluctuations in the final lipid yield, and a regulating tank should be used when necessary. In short, these results indicate the feasibility of cultivating lipid-producing microalgae in municipal wastewater for the production of biodiesel.

- **Keywords:** Scenedesmus obliquus; Biodiesel; Municipal wastewater; Primary settling tank; Secondary settling tank

Zhiguo Bian, Yingjie Li, Chunxiao Zhang, Jianli Zhao, Tao Wang, Wentao Lei. *Heat release performance and evolution of CaO particles under*

***fluidization for CaO/Ca(OH)2 thermochemical heat storage*. Pages 166-176.**

The fluidized bed reactor has been recognized for large-scale CaO/Ca(OH)2 heat storage system. In this work, the effects of critical factors such as particle size, fluidization number, steam concentration in hydration, initial temperature, cycle number and type of carrier gas on heat release performance of CaO in the fluidized bed reactor were experimentally investigated. CaO under fluidization state exhibits excellent cyclic stability on the heat release performance. The decay in heat release temperature of CaO under fluidization state is less 10% of that under static state. With increasing the cycle number, the heat release temperature of CaO using N2 as carrier gas decreases because of the rapid expansion of particles. After 20 cycles with N2 as carrier gas, the average particle size of CaO increases by 46.2% and the hydration conversion of CaO reaches above 95%. The hydration conversion of CaO experienced 20 cycles using air as carrier gas is 20% lower than that using N2 as carrier gas due to the presence of CO2 in air. The experimental investigation of CaO/Ca(OH)2 heat storage provides an important reference for the development of CaO/Ca(OH)2 system using the fluidized bed reactor.

- **Keywords:** Fluidization; CaO/Ca(OH)2 cycle; Thermochemical heat storage; Heat release temperature

Yuqing Ni, Yong Pan, Juncheng Jiang, Yinglei Liu, Chi-Min Shu. *Predicting both lower and upper flammability limits for fuel mixtures from molecular structures with same descriptors*. Pages 177-183.

Knowledge of flammability limits values, including both the lower flammability limit (LFL) and upper flammability limit (UFL), is essential to maximise safety in process design and operational procedures. This study aims to develop theoretical models for predicting both lower and upper flammability limits for fuel mixtures from molecular structures with the same molecular descriptors. All samples were collected from a single reference and the "compounds out" strategy was employed to divide the training and the test set. Descriptors for pure compounds were calculated by Gaussian 16 and Multiwfn package. The developed LFL and UFL models were validated with rigorous internal and external validations. The results indicated the robustness, validity, and satisfactory predictivity of the established models. The applicability domain (AD) of the model was also defined. The established LFL and UFL models demonstrated that the higher dipole moment and van der Waals volume are, the higher LFL and lower UFL values are. The proposed models can be expected to predict the LFL and UFL values for other fuel mixtures for which experiment values are unknown, only based on molecular structures.

- **Keywords:** Flammability limit; Quantum chemistry descriptors; Fuel mixtures; Molecular structure

Kubilay Bayramoğlu, Güner Özmen. *Design and performance evaluation of low-speed marine diesel engine selective catalytic reduction system*. Pages 184-196.

Selective catalytic reduction (SCR) systems are among the most effective methods used to reduce NOX emissions in internal combustion engines. SCR system performance is directly related to exhaust gas characteristics such as temperature and mass flow rate. Two-stroke engines commonly used in ships have different exhaust gas temperatures compared to four-stroke engines. In low-speed two-stroke diesel engines, the gas temperature drops after the exhaust gas expand in the turbocharger turbine, affecting SCR system performance. The main objective of this study is to determine performance parameters of marine SCR systems using computational fluid dynamics (CFD). The working processes of low-pressure SCR (LP-SCR) and high-pressure SCR (HP-SCR)

systems were examined comparatively. The SCR system was modeled to include urea-water solution (UWS) decomposition and catalytic reduction reactions in the study. In the designed model, the amount of injected urea-water solutions (UWS), SCR bypass valve (RBV) opening, thermolysis and hydrolysis reactions, ammonia (NH3) slip and NOX reduction performances were investigated. In addition, pressure drop, velocity distribution and optimal catalyst length were determined on the model. The results showed that an increase in UWS reduces NOX emissions however increases the probability of NH3 slip. Increasing the RBV opening also reduced the pressure loss, which was beneficial to engine performance. However, the increasing RBV opening decreased the NOX reduction performance and increased the NH3 slip. The optimal SCR catalyst length was determined as 1200 mm. Furthermore, in the studies carried out under the same boundary conditions, the HP-SCR system meets the IMO Tier III standard, but it was observed that the LP-SCR system could not meet the standard due to the decreasing temperature in the turbine.

- **Keywords:** HP-SCR; Diesel engine; UWS injection; NH3 slip; Pressure drop

Amelie Peter Affery, Jian Xiang Tan, Ian Yan Beng Ong, Juin Yau Lim, ChangKyoo Yoo, Bing Shen How, Gabriel H.T. Ling, Dominic C.Y. Foo. *Optimal planning of inter-plant hydrogen integration (IPHI) in eco-industrial park with P-graph and game theory analyses*. Pages 197-218.

With the rising demand for hydrogen in petrochemical and refineries complexes, the optimisation of hydrogen utility is getting more attention. Through inter-plant hydrogen integration (IPHI), the overall hydrogen consumption and purged gases could be further reduced by exchanging hydrogen gases among multiple plants which could reduce the climate change effect. In this work, a P-graph methodology is proposed for the optimal design of IPHI with regeneration-reuse/recycle via a centralised utility hub. Green hydrogen is incorporated in this work in the call for climate change adaption. A case study involving green hydrogen sourced from solar energy, palm oil mill effluent, and wastewater was used to demonstrate the proposed methodology. Four integration schemes were analysed using game theory-based approach for decision making. In IPHI, each participating plant may seek to maximise its own benefits due to rational self-interest. Hence, a game theory-based approach was used to analyse the interaction of participating plants in developing the IPHI schemes. With the implementation of carbon tax, it is potential for motivating collaborations as additional gains can be achieved through collaboration compared to short-sighted self-interest decision. The proposed methodology indicates that collective welfare can be maximised through cooperation among all networks to pursue Pareto optimality and in line with the commitment to tackle climate change and reaching sustainainability agenda.

- **Keywords:** Game theory; Inter-plant planning; Process optimisation; Renewable energy; Hydrogen energy; Climate change

Yue Tian, Dongfeng Zhao, Chi-Min Shu, Nitin Roy, Meng Qi, Yi Liu. *Study on thermal stability and thermal decomposition mechanism of 1-((cyano-1-methylethyl) azo) formamide*. Pages 219-229.

1-((Cyano-1-methylethyl) azo) formamide (CABN) is an azo initiator that has the inherent property of being decomposed at high temperatures with considerable amounts of heat generated. The thermal hazard of CABN is the main consideration in the occurrence of serious accidents. In this study, differential scanning calorimetry (DSC) was used to obtain the heat flow profiles and thermodynamic parameters of pure and impure CABN at various heating rates. The gaseous products and decomposition residues corresponding to each mass loss stage of CABN were judged by a thermogravimetry-mass spectrometer (TG-MS) and infrared spectrometer (IR). The optimal thermal

decomposition reaction path of CABN was simulated and determined by the Gaussian software. The Materials Studio software was used to simulate the front-line orbits and energy gaps of CABN and its mixture to determine the influence of impurities on the thermal stability of CABN. Above results showed that the addition of the impurities caused an increased thermal decomposition risk of CABN. N2, CO, CO2, CH4N2O, 2-aminoisobutyronitrile, and isobutyronitrile were the potential products as a result of the thermal decomposition of CABN. The results of this study are expected to provide the fundamentals for safely handling CABN in preparation, production, transportation, and storage purposes.

- **Keywords:** Thermodynamics; Molecular simulation; Bond dissociation energy; Thermal decomposition mechanism; Thermal stability

Ashraf Mimi Elsaid, Hany A. Mohamed, Gamal B. Abdelaziz, M. Salem Ahmed. *A critical review of heating, ventilation, and air conditioning (HVAC) systems within the context of a global SARS-CoV-2 epidemic*. Pages 230-261.

The Coronavirus disease (COVID-19) has spread over the world, resulting in more than 225 million patients, and 4.7 million deaths in September 2021. It also caused panic and terror, halted numerous activities, and resulted in the world economy deteriorates. It altered human behavior and compelled people to alter their lifestyles to avoid infection. Air conditioning systems are one of the most important sectors that must be considered because of the pandemic SARS-CoV-2 all over the world. Air is used as a heat transfer medium in heating, ventilation, and air conditioning (HVAC) systems. The air contains a variety of pollutants, viruses, and bacteria, all of which have an impact on and destroy human life. Significantly in summer, people spend more time in air conditioners which results in lower levels of vitamin D and melatonin which may affect the functioning of their immune system and are susceptible to receiving SARS-CoV-2 from other individuals. As an important component of air conditioning and ventilation systems, the air filter plays a significant role. As a result, researchers must work harder to improve its design to prevent the ultra-small particles loaded with COVID-19. This paper contributes to the design of existing HVAC systems in terms of their suitability and impact on the spread of the hybrid SARS-CoV-2 epidemic, as well as efforts to obtain a highly efficient air filter to remove super-sized particles for protection against epidemic infection. In addition, important guideline recommendations have been extracted to limit the spread of the SARS-CoV-2 throughout the world and to get the highest quality indoor air in air-conditioned places.

- **Keywords:** COVID-19 (Coronavirus) (SARS-CoV-2); Indoor air quality; HVAC; Air pollution; Ventilation; Air filter; Human thermal comfort

Maria Cristina Collivignarelli, Alessandro Abbà, Marco Carnevale Miino, Francesca Maria Caccamo, Stefano Argiolas, Stefano Bellazzi, Marco Baldi, Giorgio Bertanza *Strong minimization of biological sludge production and enhancement of phosphorus bioavailability with a thermophilic biological fluidized bed reactor*. Pages 262-276.

Identify sustainable biological sewage sludge (BSS) management represents a current challenge. In this work, pre-thickened BSS taken from a large-scale urban wastewater treatment plant (WWTP) was fed continuously for about 9 months to a semi-industrial scale thermophilic biological fluidized bed reactor (TBFBR) operating in alternate conditions. The BSS treated in TBFBR was strongly reduced (89–92%) and the production was evaluated in 0.0007–0.0023 kg kgCODremoved −1 d−1 and 0.0004–0.0014 kg kgCODremoved −1 d−1 of TS and VS, respectively. The 92% of the P-PO43- and P-org precipitated in inorganic form and accumulated in thermophilic biological

sludge (TBS). In basic soils with chelating activity, phosphorus contained in TBS presented a higher bioavailability (84.0 ± 25.3%) with respect to untreated sludge. The analysis of four diverse scenarios highlighted that TBFBR located after pre-thickening could save 73–96% of operating costs with respect to current situation.

- **Keywords:** Thermophilic fluidized bed reactor; Sludge minimization; Agricultural reuse; Circular economy; Phosphorous recovery

Haoran Zhang, Mingqi Bai, Xinyu Wang, Jianing Gai, Chi-Min Shu, Nitin Roy, Yi Liu. *Thermal runaway incidents-a serious cause of concern: An analysis of runaway incidents in China*. Pages 277-286.

China's chemical industry has experienced rapid development in the past decades. However, thermal runaway incidents have sporadically occurred, posing a serious threat to the development of the industry. This study performed the statistical analysis of 271 thermal runaway incidents that occurred in China from 1984 to 2019. Incident characteristics include the number of incidents, fatalities, spatial distributions, industry types, occurrence links, and immediate causes that were revealed and analyzed. The results demonstrated that the quantities and fatalities of incidents increased overall from 1984 to 2019. Thermal runaway incidents mainly occurred in the coastal economically developed provinces. Organic and inorganic industry accounted for 57.2% and 10.7% of the total thermal runaway incidents, respectively. According to the cause of the incidents, this study found that operator error was the biggest cause of thermal runaway, accounting for 35.4%. In addition, equipment damage, improper management, and other reasons had also led to numerous of incidents and casualties. Based upon the analysis of statistical data, this paper discussed the prevention of thermal runaway incidents in four aspects: strengthen the reliability of the process, improve the professional competence of practitioners, solve the problems of small and medium-sized enterprises, and replace passive measures for active prevention.

- **Keywords:** Thermal runaway; Statistics analysis; Chemical industry; Incident characteristics; Active prevention

Yimin Liu, Jie Ma, Lili Lian, Xiyue Wang, Hao Zhang, Wenxiu Gao, Dawei Lou. *Flocculation performance of alginate grafted polysilicate aluminum calcium in drinking water treatment*. Pages 287-294.

An inorganic-biopolymers hybrid flocculant (PSAC-SA) was prepared by modifying sodium alginate onto polysilicate aluminum calcium (PSAC) through coordination between SA and Ca2+. The preparation conditions of PSAC-SA and the flocculation parameters that influence of the turbidity and color removal efficiency were investigated and optimized. The flocculation experiments results showed that the maximum turbidity and color removal could get 97.2% and 98.4% for kaolin-humic acid suspensions, respectively. The application of PSAC-SA for Songhua River treatment indicated that it had an excellent flocculation capacity in real water samples, and its flocculation efficiency was much better than that of individual flocculants (PSAC and SA). Moreover, the flocculation mechanisms were discussed in detailed, which indicated that the bridging effect and physical entrapment of solid particles played an important role in the flocculation process.

- **Keywords:** Flocculation; Polysilicate aluminum; Sodium alginate; Drinking water treatment; Composite flocculant

Weng Fu, Harrison Hodge, James Vaughan. *Integration of fine grinding and H2SO4 leach for the liberation, dissolution and redistribution of long-life radionuclides in copper flotation concentrate*. Pages 295-305.

The economically significant deposits – iron oxide-copper-gold (IOCG) usually contains elevated amount of naturally occurring radioactive material (NORM), which hinders the utilization of IOCG deposits and leads to the waste of resources on site due to the presence of these radionuclides. Herein, a new fine grinding – H2SO4 leach method was used to efficiently dissolve and liberate long-life radionuclides (238U, 230Th, 226Ra, 210Pb, 210Po) from uranium-bearing NORM that are finely disseminated in the major economical minerals. The fine grinding treatment reduced the average particle sizes, interrupted the mineral textures and partially dissolved uranium minerals, thereby liberating them onto the newly formed secondary copper phases. The following H2SO4 leach changed the chemical and phase compositions by dissolving non-copper elements where the locked 238U and 230Th were largely removed close to the safe activity (1 Bq/g) and 226Ra, 210Pb, 210Po were mobilized onto the copper mineral surfaces. For the first time, the quantitative correlations between radionuclide species and major mineral phases were built by QXRD and radionuclide analysis. Such quantification methodology of radionuclide deportment can be applied in the processing a broad range of NORM-bearing resources, providing a crucial guidance in radionuclide management for environmental and process engineers.

- **Keywords:** Radionuclide deportment; Copper concentrate; Fine grinding; H2SO4 leach; IOCG deposit

Choong-Hee Han, ChangHee Han. *Semi-quantitative cybersecurity risk assessment by blockade and defense level analysis*. Pages 306-316.

Basically, the existing information security risk assessments use mathematics, statistics and computer science to analyze the information assets. Current academic risk assessment methodologies do not completely solve the risk from invisible cyber threats. More research and efforts are needed to fully complement the current risk assessment methodology. The most important things to be supplemented is to review the level of cyber threat blockade and level of appropriate security equipment. Unfortunately, existing methodologies are not concerned with the blockade of cyber threats and the operation of appropriate security equipment. In this paper, the new intrinsic risk assessment method by performing risk assessment is proposed in two directions. First, the risk level of the cyber threats' influx path is evaluated. Second, the level of defense systems required to treat or quarantine cyber threats that have entered inside is evaluated.

- **Keywords:** Blockade and defense level analysis; Cybersecurity risk assessment; Enhanced security control; BDLA risk management; IT risk management

Yujue Zhou, Jie Jiang, Kai Qian, Yulong Ding, Shuang-Hua Yang, Ligang He. *Graph convolutional networks based contamination source identification across water distribution networks*. Pages 317-324.

Water distribution Networks (WDNs) are one of the most important infrastructures for modern society. Due to accidental or malicious reasons, water contamination incidents have been repeatedly reported all over the world, which not only disrupt the water supply but also endanger public health. To ensure the safety of WDNs, water quality sensors are deployed across the WDNs for real-time contamination detection and source identification. In the literature, various methods have been employed to improve the performance of contamination source identification (CSI) and recent studies show that there is a great potential to tackle the CSI problem by deep learning models. The success of deep learning based CSI methods often requires a large size of training samples being collected. In real-world situations, the number of contamination events occurring in a single WDN is rather small, especially for a newly built WDN. However, the existing CSI methods in the literature mostly focus on the study of training and applying models on the same WDNs and the knowledge of CSI gained from one WDN cannot be reused by a

different WDN. To these ends, based on the application of graph convolutional networks, this paper provides a solution for cross-network CSI that can transfer the CSI knowledge learned from one WDN to a different WDN. Empirically, based on a benchmark WDN in the task of contamination source identification, we show that the proposed cross-network CSI method can achieve comparable accuracy even trained on a different WDN.

- **Keywords:** Water distribution networks; Contamination source identification; Graph convolutional network; Cross-networks learning

Xiaotong Ma, Yingjie Li, Xingkang Huang, Tai Feng, Mingfei Mu. *Sorption-enhanced reaction process using advanced Ca-based sorbents for low-carbon hydrogen production*. Pages 325-342.

Sorption-enhanced reaction process (SEPR) can produce high yield of hydrogen with in-situ CO2 removal using CaO. A key requirement for the process is the integration of effective Ca-based sorbents into catalytic schemes. In this work, the research progress of Ca-based CO2 sorbents in SEPR is summarized. The positive effects by Ca-based sorbents are analyzed. The methods to improve the reactivity of Ca-based sorbents are discussed. A good prospect of compound materials of catalysts/sorbents in SERP is pointed out, for which the relationship between the performance and structure or reaction condition should be further studied. The optimization of process parameters is critically reviewed to provide recommendations for industrial operation. The comprehensiveness of this work extends to the discussion about the applications of Density Functional Theory study in SERP. Process economics requires the integrated H2 production with by-product conversion, renewable resources utilization, waste recycling and heat coupling optimization for the future research.

- **Keywords:** Hydrogen production; CO2 separation; Sorption-enhanced reaction process; Steam reforming; CaO

Dongdong Wen, Xiaopin Guo, Rongbing Fu. *Inhibition characteristics of the electrokinetic removal of inorganic contaminants from soil due to evolution of the acidic and alkaline fronts*. Pages 343-354.

This study comprehensively investigates the inhibition characteristics of the electrokinetic removal (EKR) of inorganic pollutants from soil due to evolution of the acidic and alkaline fronts (EAAF). The effects of EAAF on the ion strength of the soil pore fluid, potential distribution, soil colloids, clay minerals, and soil microstructure are systematically examined, in addition to the control effects of non-target charged species on the removal of target pollutants. The results show that the transport of target species near the anode region is mainly inhibited by potential flattening, soil colloid aggregation, and the closure of soil pores. Migration near the cathode region is mainly inhibited by the immobile chemical states of metals, potential flattening, soil dehydration, and a high soil adsorption ability owing to the relatively developed pores. This results also show that H+, OH-, and soluble Al have a significantly control effect on the macroscopic dynamics of EKR of the target contaminants. The injection of acidic solution near the cathode alleviates the potential jump and prevents the formation of metal hydroxides to some extent. The average removal rates of nitrate, Pb, and Cd after EKR improved from 85.5%, 11.1%, and 21.8–98.5%, 35.8% and 47.7%, respectively.

- **Keywords:** Electrokinetic remediation; Soil; Inhibition; Heavy metals; Salts

Ziyuan Liao, Hexiang Yan, Zhenheng Tang, Xiaowen Chu, Tao Tao. *Deep learning identifies leak in water pipeline system using transient frequency response*. Pages 355-365.

Pipeline leak identification method using transient frequency response (TFR) has been researched in the past two decades. To extend this method to a more general water pipeline system with hydraulic uncertainties, this work (1) introduces deep learning (DL) into the TFR-based leak identification framework and (2) develops extended TFR equations in matrix form for DL learning set generation. In this framework, TFR equations are firstly solved in a pre-calibrated hydraulic model of the system to extract frequency response function (FRF) for the training set preparation. Then the simulated FRFs are fed to train fully linear DenseNet (FL-DenseNet) for feature recognition. Finally, the measured FRF of the system is fed to the trained FL-DenseNet to identify a leak to a pipe in the suspected leak area. A study on a hypothetical small system shows that the proposed framework has robustness against uncertainties of friction coefficient, wave speed, and leak flow. A significant advantage is also observed over the existing method with an inaccurate model. Then the framework is applied to a larger network. Over 90% of the synthetic leaks are identified in 5 of the 149 pipes. These results presented in the paper indicate the potential of applying this framework to a water pipeline system.

- **Keywords:** Leak identification; Deep learning; Frequency response; Water pipelines

M.D.N. Ramos, C.S. Santana, C.C.V. Velloso, A.H.M. da Silva, F. Magalhães, A. Aguiar. *A review on the treatment of textile industry effluents through Fenton processes*. Pages 366-386.

Effluents stemming from the textile industry are concerning from the environmental viewpoint, given that large volumes are generated and they present a high concentration of organic matter and toxicity. Dyes stand out among the substances present in such effluents because part of them does not fix on the fiber during the dyeing process, leaving the effluent with a strongly colored aspect and difficult to be treated. Due to the limitations and low efficiency of conventional processes, alternative forms for the treatment of textile effluents have been evaluated. Among them, the Fenton oxidation processes stand out, which are based on the use of iron as a catalyst in the conversion of H2O2 into highly reactive free radicals. The catalyst may be solubilized or used in the insoluble form (heterogeneous catalysis). Fenton reaction can be enhanced by combining UV, visible (photo-Fenton, solar photo-Fenton), or ultrasound radiation (sono-Fenton), and electrical current (Electro-Fenton). In this review, a brief mention of textile effluent characteristics is presented, and the fundamentals, advantages, limitations, and recent progress of the Fenton processes are addressed as alternatives to the treatment of textile effluents. A survey on the efficiency of such processes regarding the reduction of important characterization parameters (organic matter concentration, color, turbidity) for real textile effluents also is presented. From the real effluent data, it was noted that these processes are efficient in the reduction of organic pollutants and color. Among the Fenton processes, photo-Fenton showed better efficiencies and less variability for the different effluents treated (reducing on average 82% of COD and 95% of color). It has also been observed that such processes can be also efficient when combined with other processes (e.g. coagulation-flocculation or biological processes). Treated effluents present less toxicity and have been reused in the dyeing stage, although such an approach is still poorly evaluated. The costs for the treatment of real effluents calculated by different authors ranged from 1.1 to 28.9 USD per Kg of COD removed, where the processes that presented the lowest costs were classical Fenton and technologies that use solar energy, such Photo-Fenton and Photo-electro-Fenton.

- **Keywords:** Textile effluent; Fenton reaction; Advanced oxidation processes; Biodegradability; Toxicity; Reuse

Da Huo, Yanping Du, Heyang Wang, Jun Zhao, Wenjia Li. *Comprehensive analysis of rural heating by methanol heating stove: Economy, emissions, and energy consumption*. Pages 387-400.

Coal-fired heating, mainly used in North China, has caused serious environmental problems. Schemes to replace coal have been established, but they are not suitable for all scenarios. This paper proposes a heating scheme that uses a methanol heating stove (MHS) to meet the demand for clean, low-cost rural heating. The economy, emissions, and energy consumption of the MHS were analyzed. The scheme was compared with five common rural heating methods. The effects of the methanol price, power grid transformation, and gas pipeline construction on the annual cost of each heating scheme were investigated using a theoretical model. The MHS emitted 66 % less CO2 and 95 % less SO2 and NOx and consumed 54 % less standard coal than bulk coal heating stoves. The low electricity supply required to vaporize methanol contributed to the cost and emission reduction. Methanol price fluctuations warrant government subsidies to incentivize the implementation of the scheme. For increased adoption, we recommend that the MHS be used in areas with low population densities and methanol prices. This approach can therefore be an ideal substitute for "coal-to-electricity" and "coal-to-gas" methods in areas that lack access to power or gas supplies and can replace air-source heat pumps in severe cold zones.

- **Keywords:** Methanol heating stove; Pollutant emissions; Standard coal consumption; Methanol vaporization

Zhuang Yuan, Zhe Yang, Yiqun Ling, Chuanpeng Wu, Chuankun Li. *Spatiotemporal attention mechanism-based deep network for critical parameters prediction in chemical process*. Pages 401-414.

In chemical processes, grasping the changing trend of critical parameters can help field operators take appropriate adjustments to eliminate potential fluctuations. Thus, deep networks, renowned for its revolutionary feature representation capability, have been gradually exploited for building reliable prediction models from massive data embraced tremendously nonlinearities and dynamics. Because of the inherent complexity, the process trajectories over the whole running duration make distinctive contributions to the ultimate targets. Specifically, features extracted from different secondary variables at different previous instants have diverse impacts on the current state of primary variables. However, this spatiotemporal relevance discrepancy is rarely considered, which may lead to deterioration of prediction performance. Therefore, this paper seamlessly integrates the spatiotemporal attention (STA) mechanism with convolutional neural networks (CNN) and bi-directional long short-term memory (BiLSTM), and proposes a novel predictive model, namely STA-ConvBiLSTM. Using the deep framework composed of CNN and BiLSTM, the integrated model can, not only automatically explore the esoteric spatial correlations among high-dimensional variables at each time step, but also adaptively excavate beneficial temporal characteristics across all time steps. Meanwhile, STA is further introduced to assign corresponding weights to information with dissimilar importance, so as to prevent high target-relevant interactions from being discarded due to overlong sequences and excessive features. STA-ConvBiLSTM is applied in the case of furnace tube temperature prediction of a delayed coking unit, which exhibits a significant improvement of the prediction accuracy.

- **Keywords:** Chemical processes; Parameters prediction; Deep networks; Spatiotemporal attention mechanism; Feature representation

Jing Wu, Morten Lind, Xinxin Zhang, Karnati Pardhasaradhi, Sharat Kumah Pathi, Claus Marner Myllerup. *Knowledge acquisition and representation for intelligent operation support in offshore fields*. Pages 415-443.

Introducing Artificial Intelligence (AI) tools is one of the development trends in complex industrial systems in the industry 4.0 environment. Unique challenges in system

operations need to be handled by effective operation support systems. The knowledge-based operation support systems are developing rapidly in recent years. The paper aims at highlighting the concerns of knowledge acquisition and representation in one of the knowledge-based methodologies, the Multilevel Flow Modelling (MFM). A procedure of knowledge acquisition and representation for building MFM models is proposed to aim at improving the overall model quality and consistency. An interface linking systems' instrumentations to MFM functions are introduced. The new reasoning engine is used for MFM based real-time cause-consequence reasoning about dynamic plant situations. The model verification and validation, and the model performance evaluation analysis method are proposed. This paper also provides case studies that illustrate the effectiveness of intelligent operation support by applying MFM to an off-shore water injection system. It demonstrates that the procedure of knowledge acquisition and representation can facilitate the model builders, and ensure the quality of the models used for operation support.

- **Keywords:** Knowledge acquisition; Knowledge representation; Intelligent decision support; Offshore fields; Functional modelling

Manish Chandra Kannaujiya, Ramesh Kumar, Tamal Mandal, Monoj Kumar Mondal. *Experimental investigations of hazardous leather industry dye (Acid Yellow 2GL) removal from simulated wastewater using a promising integrated approach*. Pages 444-454.

The present investigation describes the use of bioadsorbent, ozonolysis, and integrated process (ozone integrated with bioadsorbent) treatment for leather industrial dye (Acid Yellow 2GL) removal from simulated wastewater. The morphological characterization of agriculturally based, chemically activated bioadsorbent was presented using SEM, FTIR, XRD, and BET analysis which suggested the high potential of the adsorbent for the removal from leather industry effluent. Maximum Acid Yellow 2GL removal of 98.3 ± 2.3% by integrated treatment was achieved at 30 min, bioadsorbent dose of 3 g/L and pH 7.5. Adsorption isotherms and kinetic models were measured for the validation of bioadsorption process for removal of dye. Langmuir's isotherm was best fitted for Acid Yellow 2GL dye sorption in comparison to Freundlich isotherm. The phytotoxicity analysis of treated effluent ensured that the integrated process could be a prospective candidature for the treatment of dyeing effluent from the leather industry.

- **Keywords:** Acid yellow 2GL; Bioadsorption; Integrated process; Isotherms and kinetics; Phytotoxicity

Abdhul Ahadh, Govind Vallabhasseri Binish, Rajagopalan Srinivasan. *Text mining of accident reports using semi-supervised keyword extraction and topic modeling*. Pages 455-465.

Learning from past incidents is critical to achieving and maintaining high process safety performance. Accident and incident records provide one way for learning; however, these are usually in the form of unstructured texts, which makes analysis difficult. Recently, text mining methods based on supervised learning have been proposed for analyzing accident reports; however, they require an impractically large number of labeled records as training examples. This paper proposes an automated, semi-supervised, domain-independent approach for analyzing accident reports. Given a set of user-defined classification topics and domain literature such as handbooks, glossaries, and Wikipedia articles, the method can identify domain-specific keywords and group them into topics with minimal expert involvement. These keywords and topics can then be used for various data mining purposes, including classification. The proposed approach is demonstrated using two different case studies across domains: (1) in aviation to identify the stage of flight when an accident occurs, and (2) in the process industry domain to

identify the cause of pipeline accidents. The average classification accuracy of the proposed method was 80% which is comparable to that of supervised learning methods. The key benefits of this approach are that it can generate domain-specific predictive models with limited manual intervention.

- **Keywords:** Accidents; Text mining; Document classification; Aviation Safety Reporting System (ASRS); Pipeline and Hazardous Materials Safety Administration (PHSMA)

Éverton Hansen, Jackson Kern Cardoso, Mariliz Gutterres, Patrice Monteiro de Aquim. *Scale-up testing for reducing pollution load of chemicals in wastewater of leather post-tanning*. Pages 466-472.

The leather industry has been looking for alternatives to minimize its environmental impacts, including studies to reduce the pollution load of liquid effluents from the leather process. Although studies reducing the supply of chemicals have already indicated optimized offers of fatliquoring and retanning agents, the effect of the scale-up of these optimized conditions on effluents and the quality of the leather remains unknown. This study aims to reduce the pollution load of post-tanning effluents by reducing leather chemicals supply. Tests were performed on pilot and industrial scales, reducing the offer of retanners and fatliquors in two levels: 19% and 26%. The effluents were tested for pH, conductivity, dissolved solids, sulfate, biochemical oxygen demand, and chemical oxygen demand. The leather was tested for organoleptic properties and physical-mechanical tests. The reduction of chemicals allowed the depletion of the raw wastewater pollution load. The leather obtained showed a quality within the established standards. Besides, post-tanning formulation costs were reduced by 24%.

- **Keywords:** leather chemicals; pollution depletion; retanning; fatliquoring

Lu Deng, Yang Zhang, Yiyang Dai, Xu Ji, Li Zhou, Yagu Dang. *Integrating feature optimization using a dynamic convolutional neural network for chemical process supervised fault classification*. Pages 473-485.

Chemical processes usually exhibit complex, high-dimensional, time-varying, and non-Gaussian characteristics, and the diagnosis of faults in chemical processes is particularly important. However, many current fault diagnosis methods do not consider the temporal correlation of process data, feature selection, and feature sequence arrangement. To solve this problem, this paper presents a fault diagnosis method using a dynamic convolutional neural network, based on a genetic algorithm (GA), for optimizing a feature sequence. First, the input data are transformed into a two-dimensional matrix by adding the dimension of time characteristics. Second, the GA is used to select the features, and the sequence of the selected features is optimized. Finally, the optimized feature sequence is input into the convolutional neural network (CNN) to obtain the final diagnosis results. The Tennessee Eastman chemical process is used for experimental analysis, and the proposed model is compared with the weighted cascade forest, deep belief network (DBN), optimized DBN, long short-term memory + CNN and feature selection using random forest models. The experimental results show that the proposed model has higher diagnostic accuracy. The average diagnosis rate of 20 faults is found to be 89.72%.

- **Keywords:** Fault diagnosis; Deep learning; Genetic algorithm; Sequential optimization; Convolutional neural network

Yanhui Liu, Huichang Niu, Zhao Li, Jing Liu, Cangsu Xu, Xinyan Huang. *Thermal runaway characteristics and failure criticality of massive*

***ternary Li-ion battery piles in low-pressure storage and transport*. Pages 486-497.**

Thermal runaway is a major safety concern for Lithium-ion batteries in manufacture, storage, and transport. Facing the frequent incidents in the air transport of massive batteries, more reliable fire prediction and protection strategies under low-pressures conditions are urgently needed. Herein, thermal runaway criticality of the open-circuit cylindrical battery piles (up to 9 cells with 30% SOC) under a hot boundary is investigated inside a novel low-pressure chamber (20–100 kPa). Characteristics battery temperatures for the safety venting and thermal runaway are measured to analyze the influences of pressure and cell number on battery failures. Results indicate that lowering the pressure could promote an earlier and stronger safety venting and weaken the intensity of the exothermic reactions inside cells, which is verified by the surface morphology of the electrodes. The overall fire risk is higher with higher pressure and larger battery-pile size, as indicated by the lower minimum boundary temperature for thermal runaway (255 °C~385 °C). Moreover, a simplified heat transfer model is established to explain the trend of thermal-runaway criteria and the influence of the low-pressure environment. This work delivers new insights into the effects of pressure and pile size on battery thermal runaway, which can help to improve the safe storage and transport of large-scale lithium-ion battery piles under varied pressure conditions.

- **Keywords:** Battery energy safety; Open circuit; Sub-atmospheric pressure; Cell number; Self-ignition

Yang Jun, Jiang Chenyu, Xu Zhihui, Li Mengkun, Yang Ming. *Markov/CCMT: Towards an integrated platform for dynamic reliability and risk analysis*. Pages 498-517.

An integration Markov/CCMT analytics platform for dynamic reliability and risk analysis of digital process control system is presented in the paper. The Markov/CCMT analytics platform is integrated with a simulation-based testing and matrix-based coding paradigm for automatic generation and unsupervised learning update of probabilistic mapping model and a versatile Markov/CCMT algorithm for multiway search analysis. The capabilities of the integrated Markov/CCMT analytics tool are validated with an example case study of water level control system. The results demonstrate that the features for convenient modeling, updating, and high-performance computing allows the practical and scalable use of Markov/CCMT analytics platform to risk-based reliability modeling and analysis of large complex dynamic systems.

- **Keywords:** Dynamic reliability analysis; Markov/CCMT; Multiway search algorithm; Simulation-based testing; Dynamic process system

Jianqin Zheng, Jian Du, Yongtu Liang, Chang Wang, Qi Liao, Haoran Zhang. *Deeppipe: Theory-guided LSTM method for monitoring pressure after multi-product pipeline shutdown*. Pages 518-531.

The pressure changes dramatically during the shutdown process of the multi-product pipeline. When the pipeline pressure comes to decrease, it is often mistaken as pipeline leakage or other abnormal condition which increases the burden of the operator on-site. At present, the method of pipeline shutdown pressure analysis is mainly based on numerical simulation which can not monitor shutdown pressure in real-time. In this work, the time-series approximate ability of long short-term memory (LSTM) is taken advantage of to construct a shutdown pressure prediction model. To overcome the drawback of this deep learning algorithm that is trained only by ample data, the scientific principle and theory are integrated into LSTM. Subsequently, the theory-guided long short-term memory (TG-LSTM) is proposed for pipeline shutdown pressure prediction.

The proposed model is trained with available data and simultaneously guided by the theory (physical principle and engineering theory) of the underlying problem. In the training process, the data mismatch, as well as monotonicity constraints, and boundary constraints are coupled into loss function. After acquiring the parameters of the neural network, a TG-LSTM model is established which not only fits the data, but also follows the physical principle and the engineering theory. The proposed model is verified by three real-world multi-product pipelines. The results indicate that TG-LSTM achieves better accuracy than other prediction models, with MAPE being 0.246%, 0.186%, and 0.143%, respectively. Finally, the sensitivity analysis of different hyper-parameter is conducted to illustrate the robustness of TG-LSTM in pipeline shutdown pressure prediction.

- **Keywords:** Multiproduct pipeline; Shutdown pressure prediction; TG-LSTM; Theory guided data science

Muhammet Aydin, Seher Suendam Arici, Emre Akyuz, Ozcan Arslan. *A probabilistic risk assessment for asphyxiation during gas inerting process in chemical tanker ship*. Pages 532-542.

Gas inerting process is a great hazard for chemical tanker ships and utmost care is required considering the harmful effects to humans' health. Most of the chemical tanker ship-owners face near-miss or accident (asphyxia/fire/explosion) during gas inerting process on-board ship. The consequences of the process may pose catastrophic results such as explosion, fire or asphyxiation. Therefore, a detailed risk assessment is required to enhance the process of safety during the carriage of chemical cargo and minimize potential consequences. To address this concern, the paper aims at conducting a systematic probabilistic analysis of asphyxiation risk during gas inerting process in chemical tanker ship. In the paper, a Bayesian belief network (BBN) method is used to deal with causality and uncertainty arising from the complex interdependence between variables in the probabilistic risk assessment of asphyxiation risk. While BBN enables us to calculate the conditional probability of each intermediate node and leaf node in the graph and perform probabilistic risk assessment with sensitivity analysis, fuzzy logic deals with the translation of linguistic expressions from expert opinion into probability values. The findings of the paper will provide the utmost contribution for chemical tanker ship owners, safety researchers, maritime safety professionals, and HSEQ managers (Health, safety, environment, and quality) to prevent the risk of asphyxiation during gas inerting process in maritime transportation.

- **Keywords:** Chemical tanker safety; Probabilistic risk analysis; Bayesian belief network; Asphyxiation; Gas inerting

Chenzi Teng, Jian Li. *Performance of reduction on particle emission by combining the charged water drop atomization and electric field in wet electrostatic precipitator*. Pages 543-554.

In this study, a wet electrostatic precipitator (WESP) with combination of electric field and charged water drop atomization was designed for fine particle collection, which replaced the traditional water film and mechanically spray. The removal performance was evaluated considering applied voltage, water flow rate, gas residence time, dust concentration, and continuous operation time. Results indicated that supplying charged droplets could acquire higher discharge current and better agglomeration effect than the dry type. The maximum penetration ratio was reduced from 3.8%−11.56% in the dry ESP to 3.58%−8.6% with charged droplets, as the applied voltage increased from 30 kV to 60 kV. Meanwhile, increase of water flow rate improved the total removal efficiency. The advantage of the WESP was more obvious under short gas residence time. The route of synergistically increasing gas residence time and applied voltage could largely reduce the penetration ratio, which decreased from 6.99%−19.81% to 1.03%−2.43% as they

were enhanced from 1.50 s and 30 kV to 3.33 s and 60 kV. Increasing the dust concentration led to the trend that the total removal efficiency first increasing and then decreasing gradually, resulted from combined mechanisms of particle agglomeration and suppression of corona current. Moreover, the atomization of charged water drop maintained the advantage on particle removal under continuous operation, and the efficiency drop after long-term operation could be avoided. In particular, the WESP achieved significant reduction on water consumption compared to conventional large-scale and on-site WESPs in application with equivalent levels of removal efficiency.

- **Keywords:** Wet electrostatic precipitator; Charged water drop atomization; Electric field; Combined effect; Particle removal; Water consumption

Yu Jianxing, Wu Shibo, Chen Haicheng, Yu Yang, Fan Haizhao, Liu Jiahao. *Risk assessment of submarine pipelines using modified FMEA approach based on cloud model and extended VIKOR method*. Pages 555-574.

The development of offshore oil and gas resources is inevitable for a submarine pipe network. Submarine pipeline leakage can easily escalate into a catastrophic event, causing enormous loss of life and property and environmental pollution. Therefore, it is imperative to conduct risk assessments of submarine pipelines. A failure mode and effects analysis (FMEA) is a significant method in risk analysis. However, due to the uncertainty in the risk analysis process, the assessment results may not be sufficiently accurate. In this paper, to evaluate the risk of submarine pipeline with enhanced reliability, an improved FMEA method based on cloud model and extended vlsekriterijumska optimizacija i kompromisno resenje (VIKOR) is proposed. The main contributions of this method are as follows. First, to minimize the associated linguistic uncertainties during the evaluation process, the cloud model theory is used, enabling the fuzziness and randomness to be comprehensively considered. Second, an improved synthetic dynamic weight algorithm, considering the personal status of experts as well as the agreement degree and confidence level of expert comments is proposed to strengthen the knowledge of the experts to minimize incompleteness. Third, an extended two-level risk factor hierarchy of submarine pipeline failure is established to improve the comprehensiveness of risk assessment, meanwhile, an integrated weighting method considering both subjective and objective aspects is utilized to obtain the risk factor weights, which can comprehensively reveal the risk factors' relative importance. Fourth, the VIKOR method is extended with the cloud model to determine the risk priority of failure modes, which can offer a compromise solution in the context of uncertainty. Furthermore, a case study on a submarine pipeline of the Chengbei oilfield in China is performed to illustrate the applicability of proposed approach. Sensitivity analysis are carried out to observe the robustness of the proposed method. Finally, the comparison between the obtained results and that from pre-existing methods shows that the proposed method is a more accurate and effective method for the risk assessment of a submarine pipeline.

- **Keywords:** Risk assessment; Failure mode and effect analysis; Cloud model; VIKOR; Uncertainty; Submarine pipeline

Junsheng Du, Jie Chen, Yuanyuan Pu, Deyi Jiang, Linlin Chen, Yunrui Zhang. *Risk assessment of dynamic disasters in deep coal mines based on multi-source, multi-parameter indexes, and engineering application*. Pages 575-586.

For the characteristics of high frequency and strong suddenness of dynamic disasters in deep coal mines, the traditional detection and evaluation techniques applied to shallow coal mine failed to accurately judge the risk degree of disasters. Therefore, it is of great significance to use advanced detection technologies and appropriate evaluation methods

to improve the accuracy and efficiency of risk assessment in the process of coal mining. The present paper applies the rapid detection and multi-source dynamic detection technologies used in the field of mining with the purpose of improving the reliability of detection technologies for typical dynamic disaster. In this study, the data fusion technology was used to analyze data obtained from laboratory experiments, engineering survey, detection and historical data, so as to form the final dynamic and static indicators. Then, the new combined evaluation models with time series of coal and gas outburst as well as rock burst were established respectively to carry out the comprehensive risk evaluation using the least-squares method and the time-varying weight method. After the comprehensive analysis on the results of the above two evaluation models, the risk areas of the typical dynamic disasters were judged and classified. Finally, the evaluation models were coded to build an early-warning software platform that could achieve automatic evaluation and the actual 3D visualization of coal mining areas. The early-warning software platform was applied to risk assessment of dynamic disasters in Gengcun Coal Mine in Yima City, Henan Province, China. The results of the 6-month experiment showed that the risk assessment accuracy and reliability of the proposed evaluation models was 100% and 90% respectively, which indicates that the newly developed approach is reliable and can be recommended for applying in more coal mines to improve the process safety risk control.

- **Keywords:** Risk assessment; Rock burst; Coal and gas outburst; Combined evaluation models; 3D visualization