Process Safety and Environmental Protection

Rok 2021, Volume 148

May

M.S. Gad, Mohamed A. Ismail. *Effect of waste cooking oil biodiesel blending with gasoline and kerosene on diesel engine performance, emissions and combustion characteristics*. Pages 1-10.

This work investigates the effects of blending waste cooking oil (WCO) biodiesel with gasoline and kerosene on diesel engine performance, combustion characteristics and emissions compared to fossil diesel. The properties of WCO biodiesel derived through transesterification process, are consistent with the standard limits. Kerosene and gasoline additives are added to biodiesel at ratios of 5 and 10 % by volume. Tests are carried out on a diesel engine running at 1500 rpm with various loads. The decreases in peak cylinder pressures for kerosene blends are 2 and 1.5 % for K5 and K10, respectively but for gasoline blends are 3.5 and 3% for G5 and G10, respectively about diesel oil. The thermal efficiency at full load for diesel fuel had a value of 18.5 % and reduced by 9.0, 7.0, 3.5, and 2.0 % for G5, G10, K5, and K10, respectively. The CO emissions values were reduced by 24, 31, 35, 40, and 20 % for G5, G10, K5, K10, and WCO biodiesel, respectively. HC emissions were declined by 26, 33, 38, 43, and 21 % for G5, G10, K5, K10, and WCO biodiesel, respectively. NOx emissions were increased by 31, 25, 13 and 7.5 % when using G5, G10, K5, and K10, respectively about diesel oil. The smoke emissions decreases were 30, 34, 41, and 44 % when using G5, G10, K5, and K10, respectively. WCO biodiesel blended with gasoline or kerosene can be considered good alternatives for fuels in diesel engines due to their improvements in performance parameters, combustion chracteristics as well as emissions reduction.

- **Keywords:** WCO; Biodiesel; Gasoline; Kerosene; Performance; Combustion characteristics

Zhiyuan Geng, Xinhong Li, Guoming Chen, Hongwei Zhu, Shengyu Jiang. *Experimental and numerical study on gas release and dispersion from underwater soil*. Pages 11-21.

This paper focuses on the dispersion behavior of gas released from underwater soil by using experimental and numerical approaches. A small-scale experimental system is developed and a number of release scenarios are carried out. The results indicate that the released gas breaks through the sand layer after consuming a certain amount of initial energy and enters the water in the form of bubble plumes, which is similar to the theoretical model. The plume interacts intensely with the surface and forms a fountain with a periodic change in height. The effect of leak pressure, water depth and buried depth on plume behavior and critical parameters including plume diameter, fountain

height and rise time are discussed. The experimental data are also utilized to verify the effectiveness of the presented numerical model using Eulerian-Eulerian volume of fluid (VOF) approach. The validated numerical model is subsequently employed to analyze three full-scale scenarios, and the results show good consistency with the experiments. Both the experiments and numerical models are of great value for evaluating the consequences of gas released from underwater buried pipelines and providing data and theoretical support for the subsequent risk assessment.

- **Keywords:** Subseagas release; Small-scale experiment; Gas plume; Numerical simulation

Feng Sun, Wei Xu, Guangjian Wang, Ning Shi, Zhe Yang. *Development of a hazard index for reactivity management (HIRM) in chemical process.* Pages 22-34.

The management of reactivity hazards has long been a problem in chemical process and the indexing approach is believed to be an effective solution. However, while most of the reactivity indexes do not consider the runaway scenario and are often quite rough, the assessment criteria used to judge thermal runaway does not take the type of scenario or the severity of the consequences into account. At present, there are no index system that can represent the reactivity hazards in chemical process comprehensively. Therefore, this paper has developed a hazard index for reactivity management (HIRM) in chemical processes. The reactivity hazards could be identified, evaluated and managed through nine steps defined by this method. The HIRM method is able to assess various runaway scenarios and quantify the reactivity hazards based on the consequence and probability. The consequence is rated by the damage radius which represents the damage level caused by fire, explosion, and toxic release due to reaction runaway. The probability indicates the initial event frequency, the initiation time and the controllability of the entire runaway process. The reactivity risks could then be classified by the HIRM index uniformly and comprehensively, with methods to manage the risks proposed. Six sets of equipment in the dicumyl peroxide (DCP) production unit was used as an example to demonstrate the construction of the HIRM index system. The results showed good agreement with the actual risk distribution, meaning that the HIRM method is an effective tool for the management of reactivity hazards in chemical process.

- **Keywords:** Reactivity management; Hazard index; Runaway; Cumene hydroperoxide; Dicumyl peroxide

Ali Akbar Babaei, Masoumeh Golshan, Babak Kakavandi. *A heterogeneous photocatalytic sulfate radical-based oxidation process for efficient degradation of 4-chlorophenol using TiO2 anchored on Fe oxides@carbon*. Pages 35-47.

A photocatalytic sulfate radical-based advanced oxidation process was studied to degrade 4-chlorophenol (4-CP) using persulfate (PS) catalyzing UV light and heterogeneous catalyst. In this regards, ferroferric oxide nanoparticles anchored on activated carbon (FOC) was applied as a supporter of TiO2 nanoparticles for fabricating of a recoverable photocatalyst (FOCT). Some analysis techniques including PL, UV–vis DRS, XRD, FESEM-EDS, BET, TEM and VSM were utilized to determine the optical, structural, textural and physicochemical characteristics of FOCT. The reaction mechanisms of PS activation and the generation of free radicals were described in details. Moreover, degradation intermediate products were identified and reaction pathway were proposed. It was found that photocatalytic activity and oxidation performance of pure TiO2 were improved after decoration on FOC. An excellent elimination efficiency was achieved in coupling of FOCT and UV irradiation with PS. Over 99 % of 4-CP (60 mg/L) and 49 % of TOC were removed by FOCT/UV/PS at optimum operational conditions. Furthermore, high PCP

decontamination rate (> 86 %) was obtained, even at high concentrations (100 mg/L). During consecutive five runs of catalyst use, the degradation rate was decreased slightly to 88 % with a negligible decline in Fe and Ti leaching, demonstrating the excellent reusability and durability of FOCT in oxidation process. SO4– and HO radicals were detected as main reactive species that involved in the degradation of 4-CP over FOCT/UV/PS system. Thanks to good performance and easy recovery of catalyst, FOCT/UV/PS hybrid system has a great potential for environmental remediation perspectives.

- **Keywords:** Carbon-based TiO2; Persulfate activation; 4-chlorophenol; Oxidative degradation; Magnetic ferroferric oxides

Huidong Liu, Guoren Xu, Guibai Li. *Pyrolysis characteristic and kinetic analysis of sewage sludge using model-free and master plots methods*. Pages 48-55.

The pyrolysis kinetics of two types of sewage sludge (municipal sludge and pharmaceutical sludge) were studied by thermogravimetry. The collected samples were pretreated and tested with nitrogen as carrier gas at different heating rates (10, 20, 30, and 40 °C/min) using a thermogravimetric analyzer. Model-free methods and master plots method were used to calculate the pyrolysis kinetic parameters of the samples. TG/DTG results showed that the thermal decomposition of the two types of sewage sludge may be divided into three stages (Dehydration, Decomposition, and Coking stage). The activation energies of the two kinds of sewage sludge were 366.58 KJ/mol (municipal sludge) and 268.36 KJ/mol (pharmaceutical sludge), respectively. The pyrolysis mechanism of two kinds of sewage sludge was discussed by the master plots method. The results showed that under a low conversion rate, the phase interface reaction model can better explain the pyrolysis mechanism of pharmaceutical sludge; under high conversion rate, the nucleation and growth model was more suitable. For municipal sludge, power law model was most suitable in the whole range. The pyrolysis characteristic of the samples was further studied. The results showed that the organic matter in sewage sludge can be decomposed into bio-oil and bio-gas at elevated temperatures and can be used as an attractive energy source.

- **Keywords:** Municipal sludge; Pharmaceutical sludge; Pyrolysis; Kinetics; Thermogravimetry

Adawiya J. Haider, Khalid A. Sukkar, Alyaa H. Abdalsalam, Adnan F. Ali, Salah H. Jaber, Thaer T. Abdul Ridha. *Enhancement of the air quality and heat transfer rate of an air-conditioning system using a hybrid polypropylene nanofilter*. Pages 56-66.

The design of a new air filter for air-conditioning systems needs to properly manage antimicrobial activity and heat transfer performance. In this work, a hybrid nanofilter of polypropylene coated with silver nanoparticles and multiwall carbon nanotubes (Ag-MWCNTs/PP) was prepared using a modified impregnation technique under vacuum. The results demonstrated a high dispersion of AgNPs (~18 nm) and MWCNTs on the polymer fibers. The antimicrobial activity of the nanofilters was evaluated against Salmonella enterica, Pseudomonas aeruginosa, and Staphylococcus aureus bacteria. A dramatic ability to kill all types of bacteria by 100 % was observed after adding 2 mg/mL of Ag-MWCNTs. Moreover, the pressure drop and convective heat transfer across the nanofilter were evaluated by building a special testing apparatus. The pressure drop rose with increases in the air velocity. Additionally, a high heat transfer coefficient with increases in the air velocity was achieved, with values of 52.5 and 47.3 W/m2.K for the working temperatures of 20 and 30 °C, respectively. Also, the thermal conductivity of the nanofilter was enhanced significantly by 36 %, 48 %, and 68 % at additions of 1, 2, and

3 mg/mL, respectively. The prepared nanofilter showed high efficiency, low cost, and applicability for commercial production.

- **Keywords:** Air hybrid nanofilter; Convective heat transfer; Thermal conductivity; Antimicrobial activity

Shaukat Ali Mazari, Nazia Hossain, Wan Jeffrey Basirun, Nabisab Mujawar Mubarak, Rashid Abro, Nizamuddin Sabzoi, Asif Shah. *An overview of catalytic conversion of CO2 into fuels and chemicals using metal organic frameworks*. Pages 67-92.

Abundant CO2 emissions from industries and the transportation sector cause an alarming threat to the planet due to overwhelming concerns over CO2 induced climate change. To resolve this tremendous environmental pollution, the long-term solution for CO2 mitigation exists in the conversion of CO2 into value-added products through catalysis. Among several catalysts, metal organic frameworks (MOFs) are one of the remarkable candidates for CO2 conversion into fuels and chemicals. The MOFs are molded with robust structures, high porosity, high potential of CO2 adsorption, maximum atom utilization due to high dispersion and isolation of active sites of MOFs, tunability of the metal nodes, organic ligands, etc. MOFs have been implemented for several CO2 conversion processes such as cycloaddition of CO2 to epoxides, photocatalytic CO2 reduction, electrocatalytic CO2 reduction, hydrogenation, and others. These processes convert CO2 into products like cyclic carbonates, alkyl formate, formic acid, ethanol, methanol, methane, CO, and others. This study strived to explain elaborately the formation of fuels and chemicals through different catalytic processes using MOFs. Detailed reaction conditions, catalyst chemistry, reaction mechanisms, and formation rates for alkyl formate, formic acid, methanol, ethanol, CO, and methane have been critically analyzed in present study.

- **Keywords:** Metal organic framework; CO2 cycloaddition; CO2 photoreduction; CO2 electroreduction; CO2 hydrogenation

Erlei Su, Yunpei Liang, Quanle Zou, Minghan Xu, Agus P. Sasmito. *Numerical analysis of permeability rebound and recovery during coalbed methane extraction: Implications for CO2 injection methods*. Pages 93-104.

The coal's permeability plays a crucial role in coalbed methane (CBM) extraction and coal seam CO2 sequestration. An accurate understanding of permeability rebound and recovery is therefore essential. This study establishes an improved fully coupled gas migration model for CBM extraction. The permeability rebound and recovery times as well as rebound values are proposed to accurately quantify permeability evolution during CBM extraction. The evolution of these three parameters under the influence of different factors are evaluated in detail, such as initial gas pressure, the diffusion coefficient, and the permeability. The results show that the permeability rebound and recovery times increase along with initial gas pressure and the amount over time rises rapidly under high gas pressures. As the initial gas pressure increases, the permeability rebound value decreases. However, initial diffusion coefficient and permeability have a negative trend in permeability rebound, recovery time, and rebound value. These tendencies are particularly large for low initial permeabilities and diffusion coefficients, yet the change in rebound time is smaller than the one in recovery time. Finally, inspired by the relationship between permeability rebound and gas pressure change during CBM extraction, the evolution of coal seam permeability under different CO2 injection method is discussed. A stepwise increasing-pressure CO2 injection method is also proposed, which could effectively increase the volume of CO2 sequestered and reduce project costs.

Therefore, our findings shall shed light on improving coal mine safety production and reducing greenhouse gas emission.

- **Keywords:** Coalbed methane; Permeability rebound; Numerical simulation; CO2 sequestration; Injection method

Yihan Wang, Kai Wu, Qingyu Liu, Huiyan Zhang. *Low chlorine oil production through fast pyrolysis of mixed plastics combined with hydrothermal dechlorination pretreatment*. Pages 105-114.

Fast pyrolysis of the mixed plastics (PE: PP: PS: PVC = 0.5: 0.3: 0.15: 0.05) with and without hydrothermal dechlorination pretreatment were investigated in a fixed bed reactor to determine the effects of pyrolysis parameters (temperature, carrier gas flow rate and particle size) on the distribution and the quality of the products. The results showed that high pyrolysis temperature, high carrier gas flow rate and small particle size promoted the migration of organic chlorine in condensable products to inorganic chlorine in gas products. And the optimal conditions for fast pyrolysis of mixed plastics to produce oil were the pyrolysis temperature of 500 °C, carrier gas flow rate of 40 ml/min and particle size of 0.1–0.15 mm with the maximum oil yield of 67.88 wt%. Hydrothermal pretreatment of mixed plastics has shown an excellent dechlorination efficiency of 99.9 %. Furthermore, the total yield of oil and wax was increased by 7.06 wt%, meanwhile the content of C5-C9 components in the pyrolysis oil showed an upward trend when compared with fast pyrolysis without pretreatment. Besides, the concentration of methane achieved 50.68 % due to the possible weakening effect of hydrothermal pretreatment on CC bond energy of β-position.

- **Keywords:** Mixed plastics; Fast pyrolysis; Pyrolysis oil; Chlorine migration; Hydrothermal pretreatment

Gayatri Panthi, Rishikesh Bajagain, Youn-Joo An, Seung-Woo Jeong. *Leaching potential of chemical species from real perovskite and silicon solar cells*. Pages 115-122.

Despite their many advantages, solar photovoltaic (PV) cells used for electricity generation can have negative environmental impacts. The chemicals necessary for their fabrication can be released into the environment during their disposal or following damage, such as that from natural disasters. The principle objective of this study was to assess the leaching potential of chemical species, primarily heavy metals, from perovskite solar cells (PSC), monocrystalline (MoSC) silicon solar cells, and polycrystalline (PoSC) silicon solar cells under worst-case natural scenarios. In all cases, real solar cells were used as opposed to the pure component. The toxicity characteristic leaching procedure (TCLP) was used to analyze the leachates from PSCs to determine the concentrations of major component species. The results showed that broken PSCs released Si, Pb, Al, As, and Ni under TCLP conditions; lead, a major component of PSCs, was released at around 1.0 mg/L at a pH of 4.93, from both broken and unbroken PSCs. However, the concentrations of these elements in the leachate were within the toxicity characteristic (TC) limits. Encapsulation of the PSCs inhibited the release of hazardous substances, but did not completely eliminate the release of metals. TCLP results from broken MoSCs revealed that metals leached at relatively high levels: Al: 182 mg/L, Ni: 7.7 mg/L, and Cu: 3.6 mg/L. The results from broken PoSCs indicated the release of 43.9 mg/L of Cu and 6.6 mg/L of Pb, which are higher than the TC limits. These high levels may be attributed to the welding materials used on the rear side of crystalline-Si (c-Si) solar cells. This study identifies the importance of encapsulating PSCs and the welding materials on the rear side of c-Si solar cells to minimize the release of toxic substances into the environment.

- **Keywords:** Perovskite; Silicon solar cell; Hazardous substance; Leaching test; Heavy metal

Yanting Wang, Yidong Guan, Yazhuo Li, Zhang Li, Jing Wan, Yibo Zhang, Jie Fu. *High adsorption behavior and photoregeneration of modified graphite oxide-titanium dioxide nanocomposites for tetracycline removal in water*. Pages 123-134.

To integratedly utilize adsorption technology and photocatalytic degradation for tetracycline (TTC) removal, a series of graphite oxide (GO)-titanium dioxide (TiO2) nanocomposites coupled with Sr(OH)2/SrCO3 were synthesized, of which GTiSr-81 (mass ratio = 8:1:1) exhibited potent adsorption and photocatalytic activities. Loose multilayer lamellar structure and macropore structure probably contribute to GTiSr-81's high adsorption capacity; both Sr(OH)2/SrCO3 and GO improve the photocatalytic ability of TiO2. High adsorption (96.9 %) and very small desorption (<4.6 %) of TTC on GTiSr-81 were achieved. Pseudo-second-order kinetic could well describe the TTC adsorption process onto GTiSr-81, as well as Freundlich isotherm models, demonstrating a chemical adsorption mechanism and heterogeneous surface of GTiSr-81. Thermodynamic studies showed that TTC adsorption by GTiSr-81 was a spontaneous and endothermic process. Lower solution pH and ionic strength favored the adsorption of TTC onto GTiSr-81. The photocatalytic degradation study showed that GTiSr-81 had a strong photocatalytic degradation ability for TTC, with a degradation rate of 98.1 %. Antibacterial tests of the TTC solution suggested that the antibacterial activity was only caused by TTC and had no correlation with the degradation intermediates of TTC. After five adsorption–photoregeneration cycles, the adsorption efficiency of TTC on GTiSr-81 was still as high as 83.4 %, which proved that GTiSr-81 possessed potential and substantial reuse properties.

- **Keywords:** Tetracycline; Nanocomposite; Adsorption; Photocatalytic degradation; Graphite oxide

Iman Parseh, Yaghoub Hajizadeh, Nematollah Jaafarzadeh, Gholamreza Goudarzi, Ghodratollah Shakerinejad, Ahmad Badeenezhad, Nezamaddin Mengelizadeh, Saeid Fallahizadeh. *Removal behavior of gaseous furfural using a biofilter packed with perlite, ripe compost, and oak woodchips*. Pages 135-143.

Furfural is a toxic compound that is widely used in various industries. Prolonged inhalation exposure to this pollutant, especially at workplaces, can induce detrimental health effects. Therefore it is important to remove it from the environment. The present study aimed to investigate furfural removal from polluted air streams using a biofilter system. In this regard, a 4-section biofilter packed with perlite, ripe compost, and oak woodchips was operated for a 108 day-period under different operating conditions. The effects of pH (natural and acidic), inlet concentration (18.8–81.6 mg m−3), the height of biofilter layers (4 sections), and empty bed residence times (EBRTs) of 120, 70, and 30 s on removal efficiency (RE) of the biofilter were evaluated. All sampling and measurements were performed according to standard methods. The RE values under neutral and acidic conditions were 80 and 65 %, respectively. At furfural inlet concentrations in the ranges of 18.8–21.3, 35.25–42.7, and 78.4–81.6 mg m−3, the RE values were 81, 68, and 57 %, respectively. Also, the RE values at EBRTs of 120, 70, and 30 s were 83, 73, and 61 %, respectively. About half of the total RE was related to the first section of the biofilter, where the number of bacterial (6.2 log10 CFU g-1) and fungal (5.8 log10 CFU g-1) were higher than the other sections. Due to the high RE (72 %) and low pressure drop (below 43 Pa m-1) of the biofilter, it can be concluded that biofiltration is a suitable process to remove furfural from the air.

- **Keywords:** Air pollution; Biofilter; Compost; Furfural; Woodchips; Perlite

Lili Ma, Jiaxin Wang, Jiehui Li, Yajie Pang, Jinmei He, Lei Peng, Yuangang Li, Kanshe Li, Mengnan Qu. *Intelligent composite foam with reversible tunable superwettability for efficient and sustainable oil/water separation and high-concentration organic wastewater purification*. Pages 144-157.

Design and development of robust and advanced separation materials with superwettability for efficient oil/water separation are of great interest and significance because of the increasing serious oil pollution problems. Herein, we have fabricated a copper foam-based superwettable membrane material with intelligent switchable wettability, favorable durability and corrosion resistance via a facile and scalable method. Benefitting from the synergetic effect of the well-defined hierarchical 3D porous surface structure and appropriate chemistry containing pH responsive groups, the resulting superwettable material can exhibit two distinct durable surface wettabilities via pH-triggered change of dominant functional groups on its surface. By virtue of the reversible tunable superwettability, the as-prepared material is successfully exploited for intelligent and sustainable separation of multiple oil/water mixtures, especially the complex crude oil/water mixture and high concentration organic wastewater, showing superior separation performance, favorable oil/organic solvents recoverability and durability. It is well known that the application of superwettable membranes in treating complex chemical systems has been seldom reported in current works. Therefore, it is believed that the intelligent superwettable material can be widely scaled up to various oily wastewater treatment and oil spills cleanup, which will be of great significance for practical potential applications and sustainable development of ecological environment.

- **Keywords:** Smart composite foam; Switchable superwettability; Sustainable oil/water separation; Crude oil cleanup; Organic wastewater purification

Sajjad Deyhim, Farshid Ghorbani-Shahna, Babak Jaleh, Lily Tapak. *Development of scrubber with nano-TiO2 coated packing for H2S removal*. Pages 158-168.

A pilot-scale packed-bed wet scrubber with plastic packing materials was made and experimented to control hydrogen sulfide.TiO2 nanoparticles were coated on the surface of packing to improve the hydrophilicity of scrubbing liquid to form a homogeneous liquid layer on the packing surface. Air flow rate, H2S concentration, and liquid pH were selected to evaluate their effect on scrubber removal efficiency. To evaluate and model the effects of selected variables, two separate sets of experiments were designed and conducted using response surface methodology, central composite design. The former was to model the effects of air flow rate and H2S inlet concentration on removal efficiency at natural liquid pH, and the latter was aimed at total optimization, where all three variables were evaluated. Results showed that TiO2 nanoparticles substantially increased surface hydrophilicity and hydrogen sulfide removal efficiency in natural pH and total optimization by 3.12 % and 3.63 %, respectively. Moreover, air flow rate and H2S concentration had an adverse effect on H2S removal efficiency, while liquid pH positively influenced the efficiency. The optimum removal efficiency for natural pH and total optimizations were 98.83 % and 99.93 %, respectively. The results showed that hydrophilicity of packing materials has a strong effect on hydrogen sulfide removal.

- **Keywords:** Wet scrubber; TiO2 nanoparticles; Hydrophilicity; Hydrogen sulfide

Soheil Abdpour, Rafael M. Santos. *Recent advances in heterogeneous catalysis for supercritical water oxidation/gasification processes: Insight into catalyst development*. Pages 169-184.

Supercritical water processes include supercritical water (SCW) oxidation (SCWO) and supercritical water gasification (SCWG). These are promising green technologies to address critical solid waste and wastewater management challenges, and in producing clean and renewable energy. Both SCWO and SCWG can use catalysts to improve reaction performance, such as to treat biomass at more moderate temperatures in SCWO processes, and to increase selectivity for production of more desirable gas products in SCWG processes. Heterogeneous catalysis has shown to be advantageous compared to homogenous catalysis for SCW processes. This paper reviews literature on heterogeneous catalysis applied to SCWO and SCWG process from the past decade, by focusing on catalyst preparation, characterization, and mechanisms, primarily for wastewater treatment and biogas production applications. The findings show that metal oxide catalysts such as Ag2O, CeO2, CuO, Fe2O3, MgO can enhance SCWO of biomass. On the other hand, transition metal catalysts (mainly nickel- and ruthenium-based catalysts) have been more often used for SCWG of biomass in SCW, compared to metal oxides, noble metals, zeolites, and carbon-based catalysts.

- **Keywords:** Heterogeneous catalysis; Supercritical water; Oxidation processes; Solid waste gasification; Wastewater treatment; Renewable biogas production

Kumar Raja Vanapalli, Jayanta Bhattacharya, Biswajit Samal, Subhash Chandra, Isha Medha, Brajesh K. Dubey. *Single-use LDPE - Eucalyptus biomass char composite produced from co-pyrolysis has the properties to improve the soil quality*. Pages 185-198.

The co-pyrolysis of Single-use low density polyethylene (LDPE) and Eucalyptus biomass (EuBm) can be considered as a sustainable waste management technique to produce viable byproducts. This study elucidates the effects of variable temperatures (300–600 °C), residence times (90–150 minutes), and proportions of LDPE (0.25, 0.33 (w/w)) on physicochemical characteristics of LDPE - EuBm char composites. The interference of liquified polymer coating on the surface with degradation of biomass could be the reason for low nutrient extractability of chars synthesized at 300 and 400 °C. These chars were rich in volatile matter (> 68 %) and their pores were filled with partially pyrolyzed products. Interestingly however, substantial changes in properties were observed at 500 °C due to the likely synergetic effect between the feeds. The highest plant-extractable concentrations of major nutrients (Na, K, Ca, Mg, NO3−, PO43-), electrical conductivity (4.73 mS/cm), and cation exchange capacity (50.5 Cmolc/kg) of char were observed at this temperature. The optimization through regression modeling identified 524 °C, 118 min, and 31 % (w/w) of LDPE as optimal process parameters to obtain char suitable for application in soil. Soil incubation test fortified the benefits of char to soil with 3.5 times improvement in soil fertility index at 5 % (w/w) rate of application.

- **Keywords:** Co-pyrolysis; Single-use LDPE; Eucalyptus biomass; Char composite; Optimization

Kayleigh Rayner Brown, Michele Hastie, Faisal I. Khan, Paul R. Amyotte. *Inherently safer design protocol for process hazard analysis*. Pages 199-211.

Inherently safer design (ISD) is a component of industrial safety that focusses on the elimination and reduction of hazards using four principles – minimization, substitution, moderation and simplification. Process hazard analysis (PHA) has been identified as an opportunity to explicitly consider ISD and enhance the implementation of ISD within process safety management (PSM) frameworks. The PHA technique of interest for this study was the bow tie methodology. The objective of this work was to develop a protocol to identify ISD-based barriers in bow tie diagrams. Example-based guidance was used to identify potential ISD opportunities. The protocol was validated using a case study from

Contra Costa County Health Services. Protocol validation demonstrated the ability of the protocol to identify potential ISD barriers. This protocol validation is presented in this paper. Degradation factors and controls of identified barriers, including ISD barriers, are important considerations to ensure their effectiveness. Recommended future work is further protocol validation in a predictive manner in an industrial organization.

- **Keywords:** Inherently safer design; Process hazard analysis; Bow tie analysis; Process safety management; Risk management

Reynel Martínez Castellanos, Jasmim Muniz Rodrigues Dias, Isabelli Dias Bassin, Márcia Dezotti, João Paulo Bassin. *Effect of sludge age on aerobic granular sludge: Addressing nutrient removal performance and biomass stability*. Pages 212-222.

The effect of the sludge retention time (SRT) on the stability and performance of an aerobic granular sludge (AGS) sequencing-batch reactor (SBR) on the simultaneous organic matter, nitrogen and phosphorus removal from simulated domestic wastewater was assessed in a long-term study (392 days). Operated under alternating anaerobic-aerobic conditions, the reactor was subjected to four experimental conditions: uncontrolled SRT (run I), SRT of 30 (run II), 20 (run III) and 15 days (run IV). The results showed that COD removal was kept stable and over 90 % throughout the SBR operation, regardless of the SRT. On the other hand, by allowing the sludge age to be dependent on natural solids washout by effluent withdrawal (SRT of 47–61 days), phosphate removal was substantially low (15 %), as also observed at an SRT of 30 days. Filamentous bacteria overgrowth was noticed at the later conditions, which affected the stability of the granular biomass, leading to a deterioration of its settling properties. The ratio between the sludge volume index after 30 and 5 min of settling (SVI30/SVI5) was around 0.70. Biological phosphate removal started to thrive at the sludge age of 20 days (35 %), reaching around 100 % at SRT of 15 days, at which the highest P-release/COD uptake ratio (0.14 mg P/mgCOD) and specific phosphate uptake (11.4 mgPO43−-P/(gVSS h)) were observed. Under the lowest SRT applied, the granules exhibited better structural and settling properties, with the SVI30/SVI5 ratio reaching almost 1.0. Moreover, nitrification was kept stable, and, even though nitrite build-up occurred during the SBR cycle, nitrate was the main oxidized nitrogen form in the effluent. Average COD, ammonium and total nitrogen removal amounted to 93 %, 97 % and 58 %. Cycle tests under normal and special conditions were carried out to assess specific nitrification, denitrification and phosphate uptake rates, and elucidate the key players in the biological conversions processes taking place in the AGS reactor. No phosphate uptake coupled to nitrate reduction was noticed, implying that P removal was not driven by denitrifying dephosphatation activity. To track the dynamics of important microbial functional groups, fluorescence in situ hybridization analysis was conducted.

- **Keywords:** Aerobic granular sludge; Enhanced biological phosphate removal; Nitrification; Denitrification; Sludge age

Ammar H. Elsheikh, Amal I. Saba, Mohamed Abd Elaziz, Songfeng Lu, S. Shanmugan, T. Muthuramalingam, Ravinder Kumar, Ahmed O. Mosleh, F.A. Essa, Taher A. Shehabeldeen. *Deep learning-based forecasting model for COVID-19 outbreak in Saudi Arabia*. Pages 223-233.

COVID-19 outbreak has become a global pandemic that affected more than 200 countries. Predicting the epidemiological behavior of this outbreak has a vital role to prevent its spreading. In this study, long short-term memory (LSTM) network as a robust deep learning model is proposed to forecast the number of total confirmed cases, total recovered cases, and total deaths in Saudi Arabia. The model was trained using the official reported data. The optimal values of the model's parameters that maximize the

forecasting accuracy were determined. The forecasting accuracy of the model was assessed using seven statistical assessment criteria, namely, root mean square error (RMSE), coefficient of determination (R2), mean absolute error (MAE), efficiency coefficient (EC), overall index (OI), coefficient of variation (COV), and coefficient of residual mass (CRM). A reasonable forecasting accuracy was obtained. The forecasting accuracy of the suggested model is compared with two other models. The first is a statistical based model called autoregressive integrated moving average (ARIMA). The second is an artificial intelligence based model called nonlinear autoregressive artificial neural networks (NARANN). Finally, the proposed LSTM model was applied to forecast the total number of confirmed cases as well as deaths in six different countries; Brazil, India, Saudi Arabia, South Africa, Spain, and USA. These countries have different epidemic trends as they apply different polices and have different age structure, weather, and culture. The social distancing and protection measures applied in different countries are assumed to be maintained during the forecasting period. The obtained results may help policymakers to control the disease and to put strategic plans to organize Hajj and the closure periods of the schools and universities.

- **Keywords:** COVID-19; Forecasting; Deep learning; Saudi Arabia

Dadi V. Suriapparao, Garlapati Nagababu, Attada Yerrayya, Veluru Sridevi. *Optimization of microwave power and graphite susceptor quantity for waste polypropylene microwave pyrolysis*. Pages 234-243.

Microwave power and the susceptor quantity are important operating parameters in the microwave-assisted pyrolysis. This work aims at finding the optimal power and susceptor quantity from a discrete set of microwave powers (300 W, 450 W, and 600 W) and graphite susceptor quantity (50 g, 200 g, and 350 g) to pyrolyze waste polypropylene. The effect of microwave power and the susceptor quantity on heating rate, conversion efficiency, and heat losses in pyrolysis were analyzed using a central composite design (CCD). It was observed that a higher microwave power and lower susceptor quantity yielded higher heating rates, and lower heating rates were obtained for a lower microwave power and higher susceptor quantity. For example, a very low heating rate, averaging to 8.5 °C/min was obtained for a low microwave power (300 W) and a high susceptor quantity (350 g), whereas high values of heating rate (71.7 °C/min) were obtained for a microwave power of 600 W with 50 g of susceptor quantity. For a set of microwave powers considered in this study, it was observed that the required bed temperatures were acquired faster at a low susceptor quantity compared to high susceptor quantity. The oil produced from the pyrolysis of WPP has a high heating value of 44 MJ/kg and the carbon number distribution in the range of C8 to C12. The char produced has rich carbon content (96 wt.%) and a high specific surface area (195 m2/g). Cyclo alkenes with a selectivity of 70% and monocyclic hydrocarbons with a selectivity of 49.6 % were produced at 450 W and 600 W powers respectively for a susceptor quantity of 50 g. From this study, it is found that the microwave power and susceptor quantity are the important parameters for minimizing the microwave energy requirement in the pyrolysis. The low susceptor quantity and high microwave power were found to be the best for achieving fast heating rates and low energy requirements. The microwave power significantly playing a vital role in the polypropylene pyrolysis product spectrum for value-added hydrocarbons.

- **Keywords:** Polypropylene; Pyrolysis; Microwave; Graphite; Central composite design; Oil

Vanesa Gutiérrez-Rodrigo, Pedro Luis Martín, María Victoria Villar. *Effect of interfaces on gas breaktrough pressure in compacted bentonite used as engineered barrier for radioactive waste disposal*. Pages 244-257.

In a deep geological nuclear waste repository gas can be generated by different processes. Understanding the gas transport mechanisms across the engineered and natural barriers in a repository is relevant for its security assessment, both in terms of mechanical stability and of radionuclide transport. The engineered barrier may be composed of compacted blocks of bentonite and the interfaces between these blocks might evolve into preferential fluid pathways, in particular for the gas generated around the waste canisters. Small-scale laboratory tests were performed in sound samples and in samples crossed by an interface to determine gas breakthrough pressure values after saturation and the effect on them of the interface. The FEBEX bentonite, a Spanish bentonite composed mainly of montmorillonite, was used in the tests. The gas breakthrough pressure of the saturated compacted samples increased with dry density and was higher than the swelling pressure of the bentonite. Gas breakthrough could take place either in an instantaneous or in a gradual way, the difference between both modes being the flow rate, much higher in the first case. The gas transport mechanism would be microscopic pathway dilation, with microfracturing in the case of the instantaneous episodes. A sealed interface along the bentonite did not seem to affect the breakthrough pressure or gas permeability values, since the behaviour patterns were similar in both kinds of samples, depending mostly on the bentonite dry density.

- **Keywords:** Bentonite; Gas transport; Engineered barrier; Saturation; Porosity; Interface

Tomaso Vairo, Marco Pontiggia, Bruno Fabiano. *Critical aspects of natural gas pipelines risk assessments. A case-study application on buried layout*. Pages 258-268.

The safety aspects of pipelines conveying hazardous materials are included neither under the umbrella of Seveso Directives aiming at preventing major accidents at industrial facilities, nor in other EU legislations, such as the Pressure Equipment Directive (PED). Starting from evidence that in the last decades the international natural gas market has been growing at a very high rate and continues to exhibit an increasing trend, in this paper we focus on consequences deriving from accidents on high pressure buried Natural Gas Pipelines (NGP) and related probabilities of the various outcomes. A survey on historical accidents occurred on NG pipelines in the USA, Canada and EU allowed the attainment of significant statistics concerning the main factors responsible for the accident evolution, namely failure mode, immediate and root cause, evolving scenario, degree of confinement produced by the surroundings and ignition timing. In this paper, we focus on a refined Event Tree framework, to overcome the limitations of the amply applied over-conservative IP UKOOA approach. In order to evidence the capability of the approach, the use of refined PET is exemplified by means of a real case-study of a high pressure buried NG pipeline, contrasting the actual results with those obtained by conventional methods, in terms of evolving scenario probability and damage. Conclusions are drawn about the effective application of the framework within risk assessment and the uncertainties and sensitivities in the pipeline accident modelling.

- **Keywords:** Flash fire; High-pressure pipeline; Ignition probability; Jet fire; Local and remote ignition; Natural gas

Anita Kovac Kralj. *Modification of existing processes for the use of flue gas and polyethylene waste as raw materials with an applied intelligent calculation technique*. Pages 269-276.

Raw material selection is very important in industrial production, and technical, environmentally sustainable and economic criteria must be taken into account. Purified flue gas and useless polyethylene waste are proposed for use as sustainable raw materials, thus minimizing wastes and emissions and protecting the environment. The use of flue gas in this way could reduce CO2 emissions by 1.9 106 kmol/a. This study

uses an applied intelligent calculation technique to analyze the replacement of natural gas with wastes. This technique includes applied upgrades and offers environmental benefits: •Modification of existing processes with well-known technology, using wastes as raw materials•Predicting constant applied assumptions of industrial production within effective process units with sensitivity analyses using the Aspen Plus simulator•Using mathematical calculations to determine optimal and sustainable production rates and energy and raw material consumption. The constant applied assumptions provide measurable effects on optimal sustainable product production with the same quality. This technique was tested on an industrial methanol process, replacing natural gas with purified flue gas and useless polyethylene waste. By determining constant applied production assumptions within effective reactors, a hypothetical plant could generate an additional profit of 3.8 MEUR/a.

- **Keywords:** Flue gas; Polyethylene waste; Applied assumption; Mathematical model; Retrofit

Mahmoud Mahmoudi Marjanian, Shahrokh Shahhosseini, Aminreza Ansari. *Investigation of the ultrasound assisted CO2 absorption using different absorbents*. Pages 277-288.

In this research, an ultrasound assisted CO2 absorption system using different absorbents has been investigated. Ultrasonic atomization technology is one of the efficient methods to increase gas-liquid interfacial area, thereby absorption rate. First of all, the significance of each operational parameter on the absorption rate was investigated by applying the experimental design methodology. The response surface methodology (RSM) and Box-Behnken design were employed to determine the experimental design. The analysis of variance revealed the adequacy and accuracy of the proposed models. The results indicated that among the investigated variables, the input power played more important role in the absorption rate. In addition, the absorption rate was not sensitive to the temperature. Moreover, a comparative study using water absorbent indicated that applying ultrasonic atomization led to five times faster CO2 absorption rate compared to the conventional stirring method and 20 times faster rate compared to the silent condition (no ultrasonic and no stirring).

- **Keywords:** CO2absorption; Interfacial area; Ultrasonic atomization; Response surface methodology (RSM); Stirring method

Bei Pei, Zhiyin Zhu, Shuangjie Yang, Shuangming Wei, Rongkun Pan, Minggao Yu, Liwei Chen. *Evaluation of the suppression effect on the flame intensification of ethanol fire by N2 twin-fluid water mist containing KQ compound additive*. Pages 289-298.

Water mist is one of the important substitutes of halon fire extinguishing agents with the advantages of clean and environmental protection. However, there will be a short time of flame intensification in the fire extinguishing progress of water mist, which threatening the safety of surrounding combustibles and fire fighters. The main objective of this study is to assess the suppression performance of N2 twin-fluid water mist containing KQ compound additive (composed of 6% fluorine surfactant and K2CO3) on ethanol pool fire, and analyze the suppressing mechanism on the flame intensification phenomenon. Experimental results showed that: the fire extinguishing time of several fire extinguishing agents from low to high was N2 twin-fluid water mist containing KQ compound additive < N2 twin-fluid water mist containing potassium additives < N2 twin-fluid water mist < N2 twin-fluid water mist containing 6% fluorine surfactant < air twin-fluid water mist. Comparing to air twin-fluid water mist, there was no obvious intensification phenomenon of flame in the initial extinguishing stage with N2 twin-fluid water mist containing KQ compound additive, and the suppression effect on the fire was improved significantly. N2

played a pre-inerting role, which could increase the specific heat of the mixture and dilute the concentration of oxygen, resulting in reducing the flame intensity and flame buoyancy. Meanwhile, comparing to potassium salt solution, the compound additive of KQ solution reduced the droplet diameter of water mist, which fastening the generation rate of K ions; and leading to smaller turbulence disturbance on flame caused by water mist. Therefore, the physical and chemical fire extinguishing effects were both improved. Moreover, compound additive KQ reduced the potassium salt concentration by 50 %, hence reduced the corrosion of chemical additives. This research will improve the fire extinguishing efficiency and reliability of water mist fire extinguishing technology.

- **Keywords:** Ethanol fire; N2 twin-fluid water mist; Potassium salt additive; Fluorine surfactant

Lipeng Wang, Fang Yan, Fang Wang, Zijun Li. *FMEA-CM based quantitative risk assessment for process industrie: a case study of coal-to-methanol plant in China*. Pages 299-311.

Coal-to-methanol enterprises in China face many risk factors that pose a serious threat to the safety of the company's production. Therefore, it is imperative to conduct risk assessments of coal-to-methanol plants. A failure mode and effects analysis (FMEA) is a significant analysis method in risk evaluation. However, due to the uncertainty in the risk analysis process, the assessment results may not be sufficiently accurate. To reduce the uncertainty, especially randomness and fuzziness in the evaluation process, a cloud model (CM) is utilized to improve the FMEA, and the FMEA-CM approach is proposed. First, the qualitative language terms are converted into the quantitative numerical characteristics of the cloud model, enabling the fuzziness and randomness in the evaluation process to be comprehensively considered. Second, the cloud weights of S, O and D are calculated by using the interval analytic hierarchy process (IAHP) and the CM. Moreover, the cloud risk priority number (CRPN) is put forward to improve the accuracy of the traditional RPN, and the CRPN algorithm is given. Finally, to rank risk events, the technique for order preference by similarity to an ideal solution (TOPSIS) method, improved by cloud distance based on Hamming distance, is put forward. A coal-to-methanol plant in Yinchuan, China, is introduced to demonstrate the applicability of the proposed FMEA-CM approach. Compared with the results obtained from the traditional FMEA and fuzzy TOPSIS method, the results obtained from the adoption of the FMEA-CM approach show that the FMEA-CM is a more accurate and effective method for the risk assessment of a coal-to-methanol plant.

- **Keywords:** Quantitative risk assessment; Failure mode and effects analysis; Cloud model; Cloud risk priority number; Coal-to-methanol plant

Gyula Dorgo, Ahmet Palazoglu, Janos Abonyi. *Decision trees for informative process alarm definition and alarm-based fault classification*. Pages 312-324.

Alarm messages in industrial processes are designed to draw attention to abnormalities that require timely assessment or intervention. However, in practice, alarms are arbitrarily and excessively defined by process operators resulting numerous nuisance and chattering alarms that are simply a source of distraction. Countless techniques are available for the retrospective filtering of alarm data, e.g., adding time delays and deadbands to existing alarm settings. As an alternative, in the present paper, instead of filtering or modifying existing alarms, a method for the design of alarm messages being informative for fault detection is proposed which takes into consideration that the occurring alarm messages originally should be optimal for fault detection and identification. This methodology utilizes a machine learning technique, the decision tree classifier, which provides linguistically well-interpretable models without the modification of the measured process variables. Furthermore, an online application of the defined

alarm messages for fault identification is presented using a sliding window-based data preprocessing approach. The effectiveness of the proposed methodology is demonstrated in terms of the analysis of a well-known benchmark simulator of a vinyl-acetate production technology, where the complexity of the simulator is considered to be sufficient for the testing of alarm systems. Note to practitioners: Process-specific knowledge can be used to label historical process data to normal operating and fault-specific periods. Alarm generation should be designed to be able to detect and isolate faulty states. Using decision trees, optimal "cuts" or alarm limits for the purpose of fault classification can be defined utilizing a labelled dataset. The results apply to a variety of industries operating with online control systems, and especially timely in the chemical industry.

- **Keywords:** Alarm management; Alarm limit design; Fault detection and identification; Data model; Data mining

Seungkyoo Pak, Chankyu Kang. *Increased risk to people around major hazardous installations and the necessity of land use planning in South Korea*. Pages 325-333.

Risk management of major hazardous installations (MHIs) is a principal concern due to chemical hazards, both in South Korea and in foreign countries where chemical plants are located. To cope with these risks, various regulatory schemes have been developed for the recognition, prevention, and control of chemical accidents. Despite these efforts, the worst major accident caused by massive (20 t) leakage of anhydrous hydrogen fluoride occurred in Gumi City in 2012. As a result, the location of MHIs associated with the chemical industry became a major concern among the public, relating to the risks to both the public and environment. In this study, the regulatory systems in South Korea are compared with global standards for controlling major hazards, and the adoption of land use planning (LUP) is discussed. Based on population statistics for the last 17 years, the EPA's ALOHA software was used to evaluate the impact of land development and population growth around MHIs through case studies of societal risk changes at five water-treatment plants using Cl2 (chlorine). The total risk at the Cl2 sites increased by up to 3.05 times from 2000 to 2017, demonstrating the necessity of introducing LUP.

- **Keywords:** Risk management; Chlorine; Major hazard installation; ALOHA; Land use planning

Qin Xu, Shengqiang Yang, Wenming Yang, Zongqing Tang, Wanxin Song, Buzhuang Zhou, Xiaoyuan Jiang. *Effect of particle size and low-temperature secondary oxidation on the active groups in coal structures*. Pages 334-344.

To analyze the secondary oxidation of the active structures of pulverized coal and reduce risks of coal spontaneous combustion, free radical theory and functional group analysis were combined to study the effects of particle size and oxidation temperature on the active structure of coal molecules. This process was based on electron paramagnetic resonance (EPR) and Fourier-transform infrared (FTIR) technology. The results show that the reduction in pulverized coal particle size can enhance the secondary oxidation activity of coal and that the reactivity is the strongest when the particle size is 0.074−0 mm. The smaller the coal particle size is, the shorter the aliphatic side chain is after secondary oxidation. The reaction in which the side chain breaks to form a stable chain structure is also more intense. A smaller coal particle size also makes it easier to produce −OH after secondary oxidation, resulting in a large increase in the Average A (−OH) in the Coal 1# and Coal 3# at the minimum particle size range of 0.074−0 mm. The −C=O and −C−O− in Coal 1# with a lower metamorphic grade are greatly affected by temperature and particle size, and the consumption of −C=O during oxidation plays a dominant role in the

secondary oxidation process. The −C=O and −C−O− in Coal 2# and Coal 3# are less affected by temperature and more affected by particle size, and −C−O− is the main group driving the secondary oxidation reaction.

- **Keywords:** Free radical; Functional groups; Oxidation temperature; Spontaneous combustion disaster; Safety production process

Indrajit Ghosh, Sayanti Kar, Tamasha Chatterjee, Nirjhar Bar, Sudip Kumar Das. *Removal of methylene blue from aqueous solution using Lathyrus sativus husk: Adsorption study, MPR and ANN modelling*. Pages 345-361.

The low-cost, eco-friendly husk of Lathyrus sativus(HLS) was tested as a promising bio-sorbent for removing methylene blue (MB) dye from aqueous solution. The batch study was conducted to remove toxic MB dye using untreated (UHLS), and acid-treated husk, i.e., 1 N H2SO4 treated (SHLS) and 1 N H3PO4 treated (PHLS). The BET, FTIR, SEM, and pHPZC are used to characterize the adsorbents. The effects of operating parameters like dye concentration, pH, contact time, temperature, and adsorbent dose on the adsorption process were investigated. The maximum adsorption capacity of UHLS, SHLS and PHLS adsorbents are 98.33 mg/g, 104.28 mg/g and 113.25 mg/g respectively at 303 K temperature. However, at elevated temperature maximum adsorption capacity is decreased. The removal percentage was more than 99 %. The Langmuir and Temkin isotherm model was well fitted for all the adsorbents at 313–323 K.The pseudo-second-order kinetic model has been the best fit. The sorption energy calculated by using D-R isotherm showed the physical adsorption process. The negative integer of thermodynamic parameters(ΔG°, ΔH°, and ΔS°) indicated that the adsorption process was exothermic, spontaneous, and decreased disorder at higher temperature.50 % glacial acetic acid was found to be the best desorbing agent for the MB loaded adsorbents. The MPR and also ANN techniques have predicted dye removal very successfully with a high degree of accuracy.

- **Keywords:** Acid treatment; Adsorption; Desorption; Husk of Lathyrus sativus; Methylene blue dye

Ke Gao, Shengnan Li, Yujiao Liu, Jinzhang Jia, Xiaoqi Wang. *Effect of flexible obstacles on gas explosion characteristic in underground coal mine*. Pages 362-369.

Gas explosion is one of the fatal accidents in underground coal mine, threatening the lives of miners and causing significant economic losses. Gas explosion characteristics are affected by many factors, including flexible obstacles such as flexible duct systems (DS) and line brattices (LB) in the auxiliary ventilation system. In order to explore the influence of flexible obstacles in the tunnel on the propagation law of gas explosion, this study established a numerical simulation model by using OpenFOAM that is an open-source CFD source code. The process variable in XiFoam tools was used for deflagration reaction. Gas explosion simulations were carried out for analyzing the impacts of DS and LB on the evolution of flame and shock wave propagation inside the tube. The results showed that the effect of flexible obstacles on the flame propagation law was evident. The flame shape easily caused many wrinkles in the tube with flexible obstacles. Meanwhile, the maximum pressure and flame propagation speed changed obviously comparing with the empty tube. In the model of DS and LB, the maximum pressure increased by 29 % and 77.8 % than the maximum pressure of empty tube, and the maximum flame propagation speed increased by 6.8 % and 20 % than the flame propagation of empty tube, respectively. The results can provide guidance for gas explosion prevention in underground coal mine.

- **Keywords:** Flexible obstacle; OpenFOAM; Gas explosion; Coal mine

Yekai Yang, Chengqing Wu, Zhongxian Liu, Jianmei Du, Hai Zhang, Shenchun Xu, Shaoqiang Zhou. *Protective effect of unbonded prestressed ultra-high performance reinforced concrete slab against gas explosion in buried utility tunnel*. Pages 370-384.

With the wide application of natural gas, in order to increase the sustainability of buried utility tunnel and prevent the explosion of the gas pipeline cabin from threatening process safety, the performance of the partition wall (slab) of the cabin against gas explosion should be investigated. This paper presents the protective effect of unbonded prestressed ultra-high performance reinforced concrete slab (UPUHPRCS) against gas explosion in buried utility tunnel. There were four scenarios in the experiment, among which the variables were the length of tunnel (12,000 mm and 20,000 mm) and gas concentration (7.5 % and 9.5 %). The normal strength reinforced concrete slab (NSRCS) and ultra-high performance reinforced concrete slab (UHPRCS) were tested as reference specimens, and the simple supported steel slab fixed by stacking sandbags was compared with the concrete slab fully constrained on the tunnel. The overpressure curves caused by gas explosions in the tunnel, the damage of each concrete slab and the change of deflections were obtained through the tests. The results indicated that with the increase of the length of the buried utility tunnel, the power of gas explosion will further increase, and the UPUHPRCS, as the partition wall of the gas pipeline independent cabin in the buried utility tunnel, will play an excellent role in against gas explosion. Moreover, the gas explosion may have little effect on the circular section pipeline in the independent cabin.

- **Keywords:** UHPRCS; UPUHPRCS; Gas explosion; Buried utility tunnel; Overpressure

Yanhui Li, Shuzhong Wang, Tongtong Xu, Jianna Li, Yishu Zhang, Tiantian Xu, Jianqiao Yang. *Novel designs for the reliability and safety of supercritical water oxidation process for sludge treatment*. Pages 385-398.

For strengthening the safety and reliability for supercritical water oxidation (SCWO) process, the essential causes and solutions of key challenges such as the high corrosion risk of the heat-exchanger and the entrance part of SCWO reactor, the blockage problems resulted from the solid deposition, and the safety and environmental issues caused by the emergency discharge of supercritical aqueous fluids, were investigated theoretically and experimentally. The thermodynamic state division between chemical- and electrochemical corrosion and the corrosion sensitive temperature range of 280−450 °C featuring the predominant electrochemical corrosion were proposed. A set of optimized parameters for the petrochemical sludge treatment such as a temperature of 520–580 ℃, a pressure of 23−25 MPa, and an oxidation coefficient of 1.1–1.3, which not only can ensure the high enough removal rate of organic pollutants but also prevent the corrosion of construction materials as much as possible; the critical velocity of conveying fluid for avoiding the deposition of solid particles were also obtained. On the bases of innovatively developing the "indirect heat transfer" unit, the mixing-preoxidation equipment, the oxygen removal process for SCWO effluents, and the emergency discharge protection device, a novel SCWO process and its corresponding control scheme were proposed and analyzed.

- **Keywords:** Supercritical water oxidation; Sludge treatment; Process safety; Process design; Corrosion prevention; Emergency discharge

A. Ewees. *Efficient artificial intelligence forecasting models for COVID-19 outbreak in Russia and Brazil*. Pages 399-409.

COVID-19 is a new member of the Coronaviridae family that has serious effects on respiratory, gastrointestinal, and neurological systems. COVID-19 spreads quickly worldwide and affects more than 41.5 million persons (till 23 October 2020). It has a high hazard to the safety and health of people all over the world. COVID-19 has been declared as a global pandemic by the World Health Organization (WHO). Therefore, strict special policies and plans should be made to face this pandemic. Forecasting COVID-19 cases in hotspot regions is a critical issue, as it helps the policymakers to develop their future plans. In this paper, we propose a new short term forecasting model using an enhanced version of the adaptive neuro-fuzzy inference system (ANFIS). An improved marine predators algorithm (MPA), called chaotic MPA (CMPA), is applied to enhance the ANFIS and to avoid its shortcomings. More so, we compared the proposed CMPA with three artificial intelligence-based models include the original ANFIS, and two modified versions of ANFIS model using both of the original marine predators algorithm (MPA) and particle swarm optimization (PSO). The forecasting accuracy of the models was compared using different statistical assessment criteria. CMPA significantly outperformed all other investigated models.

- **Keywords:** COVID-19; Optimization; Chaotic marine predators algorithm; Forecasting; Artificial intelligence; Russia; Brazil

Tianlong Zheng, Lin Li, Fengguang Chai, Yanjie Wang. *Factors impacting the performance and microbial populations of three biofilters for co-treatment of H2S and NH3 in a domestic waste landfill site*. Pages 410-421.

Numerous volatile organic compounds and odors are generated when municipal solid wastes decompose in landfill sites. Three biofilters (BF-1, BF-2, and BF-3) were deployed to remove H2S and NH3 accumulated under high density polyethylene films in a 30,000 m2 area landfill site in North China. Results showed that the inlet concentrations of H2S and NH3 were 16.4–220.3 mg/m3 and 2.0–56.4 mg/m3, respectively. Outlet concentrations were reduced to 1.0–33.1 mg/m3 for H2S and 0–9.2 mg/m3 for NH3. The H2S removal efficiencies were around 91.1 % for BF-1, 87.0 % for BF-2, and 82.6 % for BF-3 in a steady state. The respective removals of NH3 were 92.0 %, 89.3 %, and 81.1 %. Thus, H2S and NH3 were both treated effectively by the biofilters. The intake load presented a seasonal variation. A high elimination capacity was obtained in the biofilter harvesting high inlet load. High throughput sequencing technology was utilized to assay the microbial populations in the biofilters. Pseudomonas sp., Alicyclobacillus sp., Sphingomonas sp., and Rhodanobacter sp, which were linked to the degradation of H2S and NH3, were isolated and identified. Their characteristics and distributions in the biofilters depended on the inlet concentration of substrates and the microenvironment within the packing materials. The results from this bio-product analysis indicated that most of H2S was bio-oxidized into sulfur and sulfate while NH3 was converted into nitrate or dissolved into the liquid phase mainly by absorption or chemical neutralization in the biofilters.

- **Keywords:** Landfill site; Odour removal; Biofilter; Performance; Microbial population; Conversion pathway

Kun Chen, Xin Wei, Hui Li, Hao Lin, Faisal Khan. *Operational risk analysis of blowout scenario in offshore drilling operation*. Pages 422-431.

Offshore drilling is a complex and hazardous operation. The safety of the drilling operation is a strong function of many time-dependent parameters. The traditional risk analysis model fails to capture the impact of spatial and temporal variations of these parameters. This paper presents a Bayesian Network (BN) model for the offshore drilling

operation. The model uniquely considers the evolution of hazards as a function of time and space, and failure of the safety barriers. The model development is explained using the bowtie approach, which is routinely used in the industry for risk management. The bowtie model is subsequently transformed into a BN model and simulated for the well blowout scenarios. The blowout risk is updated based on operational field observations. An uncertainty analysis is also conducted to capture the spatial variability of the parameters. The results of the BN model provide a dynamic risk profile of the blowout accident during the drilling operation. Other possible accident scenarios, such as lost circulation, can also be analyzed using the proposed model. The proposed BN model serves as a robust tool for risk management of offshore drilling operations.

- **Keywords:** Drilling blowout; Dynamic risk analysis; Bow-tie model; Bayesian, probability updating; Offshore safety; Data-driven model

Sajjad Adhami, Ahmad Jamshidi-Zanjani, Ahmad Khodadadi Darban. *Remediation of oil-based drilling waste using the electrokinetic-Fenton method*. Pages 432-441.

The large amount of residues and pollutants left over from the drilling industry could cause irreparable damage by entering the human and animal food chain. Therefore, drilling waste management is of particular importance. Electrokinetic (EK) remediation is one of the methods used to remediate all types of soils contaminated with metal and organic pollutants, but the special conditions and properties of drilling wastes make the use of this method more complex for the treatment of this type of waste. In this study, by enhancing the EK method with Fenton technique, which is an advanced oxidation technique, and using copper and iron electrodes as anode, total petroleum hydrocarbons (TPH) were removed from the oil-based drilling waste. The best result in this study was obtained by reducing the initial concentration of TPH from 316,000 to 72,680 mg/kg in drilling waste. This 77 % reduction in TPH concentration was achieved using the EK method coupled with Fenton technique along with the use of copper electrode. The use of iron electrode in the EK-Fenton (EK-F) method improved the parameters affecting the removal efficiency and pollutants decomposition and resulted in 69.6 % TPH removal. These results show a 161 % (copper) and 136 % (iron) increase in TPH removal efficiency, respectively, compared to the conventional EK method, in which TPH removal was 29.4 %. These results indicate that the use of EK-Fenton method combined with copper electrode is effective in removing TPH from drilling waste. Overall, the promising results of the present study indicate that the enhanced EK technique could be considered as an effective and environmentally friendly approach for the drilling waste remediation.

- **Keywords:** Drilling; Hazardous waste; TPH; Electrokinetic; Fenton

Ascendino P. de Araújo Neto, Fabricia A. Sales, Wagner B. Ramos, Romildo P. Brito. *Thermo-environmental evaluation of a modified Waelz process for hazardous waste treatment*. Pages 442-450.

Electric arc furnace dust is a waste by-product of electric arc furnaces in steel production. This material is hazardous to the environment due to the presence of metals, such as chromium, lead, and cadmium; in addition to these, there is zinc in its composition. One of the main ways of recovering zinc from the electric arc furnace dust is carried out in rotary kilns called Waelz kilns. This work aims to develop a model of a Waelz kiln and evaluate the impact of processing sludge from an industrial effluent treatment plant as a feed along with electric arc furnace dust, with and without the inclusion of a drying system for the sludge and a thermal integration system with the Waelz slag. The model, validated against industrial data plant, revealed an optimum operational point, resulting in a zinc recovery of 98.3 %, which is equivalent to an increase in the production by 6.2 %. The scenario with direct sludge feed into the kiln resulted in a maximum zinc recovery rate of 89 %. The results from the sludge drying scenario imply a zinc recovery of 94 %

and represent a viable alternative for reducing the amount of solid waste generated in the zinc production plants that use the Waelz kiln by 1100 t/year per tonne of sludge treated. Furthermore, it also increased zinc production to 1300 t/year.

- **Keywords:** Zinc oxide; Electric arc furnace dust; Waelz kiln; Thermal integration; Dryer system

Saleh Abo-Elfadl, Mohamed S. Yousef, Hamdy Hassan. *Energy, exergy, and enviroeconomic assessment of double and single pass solar air heaters having a new design absorber*. Pages 451-464.

This paper experimentally examines the performance of solar air heater (SAH) having a newly designed tubular absorber comprising adjacent parallel tubes called tubular SAH (T_SAH) via energy, exergy, and enviroeconomic standpoints. A comparative performance assessment between T_SAH and flat plate solar air heater (F_SAH) at diverse air mass flow rates (MFRs) of 0.075, 0.05, and 0.025 kg/s is performed. Experiments for both heaters are tested using two flow pass arrangements of single-pass (SP) and double-pass (DP). The results reveal that maximum enhancement in thermal and exergy efficiencies of 133 % and 330 %, respectively is obtained when using SP T_SAH against SP F_SAH at air MFR of 0.025 kg/s. It is found that when there is an increase in air MFR, there is a significant increment in thermal efficiency, whereas there is a reduction in exergy efficiency. Despite the performance in the case of T_SAH is more effective than F_SAH, the enhancement in the case of DP F_SAH due to using DP flow configuration is greater than that of DP T_SAH. Finally, the results indicate that the carbon credit earned regarding the amount CO2 mitigated for SP F_SAH and SP T_SAH at MFR of 0.075 kg/s is estimated at 391.6 $/year and 561.9 $/year, respectively.

- **Keywords:** Tubular SAH; Flat SAH; Energy and exergy; Double and single-pass; Environmental

Chao Chen, Shaokang Qu, Mengli Guo, Jie Lu, Weiming Yi, Ransheng Liu, Jincheng Ding. Waste limescale derived recyclable catalyst and soybean dregs oil for biodiesel production: Analysis and optimization. Pages 465-475.

The focus of this work is to develop a reusable heterogeneous catalyst for the preparation of biodiesel. Among the potential raw materials, soybean dregs oil is extracted from waste soybean dregs, and limescale is used as a source of calcium oxide. The basic catalyst of mixed metal oxide of CaO and Al2O3 was synthesized by sol-gel method. The structure, composition and basicity of the synthesis catalyst were characterized by TG, XRD, BET, SEM-EDX, TEM-EDX, FTIR and CO2-TPD. The results indicate that the presence of the inert substance Ca5Al6O14 inhibits the accumulation of CaO and promotes its dispersion uniform. The FAEE yield reaches 92.6 % under the optimized conditions. Kinetic analysis shows that the experimental pattern conforms to a pseudo-first-order reaction kinetic model (R2 = 0.9674), and the activation energy required for the transesterification reaction is Ea = 62.36 KJ/mol. In addition, the catalyst shows high stability in this experiment, and no obvious performance loss is observed during the process of five cycles.

- **Keywords:** Limescale; Soybean dregs oil; Ca5Al6O14; Biodiesel; Transesterification

Francisco J. Navarro-Gonzalez, Yolanda Villacampa, Miguel Ángel Pardo Picazo, M. Cortés-Molina. *Optimal load scheduling for off-grid photovoltaic installations with fixed energy requirements and intrinsic constraints*. Pages 476-484.

Solar energy is one of the most promising green energy sources. On-grid photovoltaic installations supply energy to consumers as a support energy source, but in isolated areas, it comes as the unique source. The decision-maker must dimension the installation, maintaining system performance with reasonable investments. In some scenarios, the utility manager can handle the energy delivered to consumers as every subsystem can be independently connected. A strategy for scheduling the energy consumption to decrease the number of photovoltaic modules required in a standalone system is proposed here. The problem formulation corresponds to generalising a more specific problem before published. We presented a real case study being the groups of hydrants that provide water to crops in a pressurized irrigation system for energy consumption to schedule.

- **Keywords:** Energy efficiency; Photovoltaic energy; Solar plant size optimization

Kumaran Shanmugam, Musab Abdul Razak. *Assessment on process safety management implementation maturity among major hazard installations in Malaysia*. Pages 485-496.

Despite the widespread process safety management (PSM) implementation among major hazard installations (MHI) in Malaysia, an assessment on current PSM implementation maturity had never been conducted. This study aims to provide such assessment, through the utilisation of PSM elements under the OSHA PSM standard. The study first involved the measurement of PSM implementation achievement grades as well as, the development of PSM implementation related process safety maturity model and process safety assessment rubrics. Both the achievement grades and maturity model were then utilised for the assessment on PSM implementation maturity among MHI in Malaysia. Suitable recommendations for improvements in effectiveness of PSM implementation were finally proposed with reference to the assessment rubrics. From the individual PSM elements implementation assessment results, the Pre-Startup Safety Review element registered the highest representative percentage of 24 %, of MHI in Malaysia having PSM implementation maturity below the predefined acceptable maturity levels. From the overall PSM implementation assessment results, it was found that a representative percentage of 40 % of MHI in Malaysia displayed PSM implementation maturity below the similar predefined acceptable maturity levels. However, the study emphasised that future improvements to the PSM implementation maturity could be achieved through the implementation of the proposed recommendations.

- **Keywords:** Process safety management; PSM implementation assessment; Maturity model; Major hazard installation; Assessment rubric

Krishnasamy Sivagami, Govindaraj Divyapriya, Ramya Selvaraj, P. Madhiyazhagan, N. Sriram, Indumathi Nambi. *Catalytic pyrolysis of polyolefin and multilayer packaging based waste plastics: A pilot scale study*. Pages 497-506.

The catalytic pyrolysis of different types of polyolefin and multilayer packaging based plastic wastes in the presence of commercial zeolite catalyst was studied in the batch pilot scale reactor. Different types of multi-layer plastics such as biaxial oriented polypropylene (BOPP), metalized biaxial oriented polypropylene layers (MET/BOPP), poly ethylene terepthalate (PET), metalized polyethylene-terepthalate (MET/PET), PET combined polyethylene (PET/PE) and mixed polyolefin plastic wastes obtained from the municipal corporation were pyrolyzed to determine the oil, gas and char distribution. BOPP based plastic waste exhibited higher oil yield and calorific value (65–70%, 45.14 KJ/g) compared to PET based MLPs (17.8 %, 30 KJ/g) and laminated metalized plastics (13 %, 37 KJ/g). Modifying the feed composition by mixing of polyolefins-based waste plastics with PET based MLPs and BOPP/MET BOPP doubled the liquid yield and notably

altered the physicochemical characterization of the resulted pyrolysis oil. Char yield in the polyolefins-based waste is observed to be lesser than the MLP based waste plastics. GC–MS analysis revealed the percentage area of hydrocarbons compounds of the pyrolysis oil obtained from PET based MLP experiments contains high fractions of medium and heavier range hydrocarbons (C11 – C20, C21 – C30). Sulfur content in the oil from different MLPs was measured as below the detection limit. Functional groups of hydrocarbons of oil were analyzed using FT-IR. Solids were characterized for the presence of heavy metals such as Al, Cr, Cu, Co, Pd, and Ni.

- **Keywords:** Catalytic pyrolysis; Polyolefin plastic waste; Multilayer plastics; Zeolite; Fuel oil; Char

Til Baalisampang, Elie Saliba, Fatemeh Salehi, Vikram Garaniya, Longfei Chen. *Optimisation of smoke extraction system in fire scenarios using CFD modelling*. Pages 508-517.

Understanding the consequences of fuel release and fire accident is an important aspect of the design and construction of buildings and infrastructures. Particularly, an increasing number of catastrophic consequences of recent fire accidents in high-rise buildings has led to the demand for a rigorous and holistic approach for infrastructure fire safety analysis and performance evaluation. The current study proposes a framework for liquefied petroleum gas heat release simulations and modelling the visibility of evacuees on the egress path during a fire event using efficient computational fluid dynamics (CFD) model. The framework consists of scenario modelling, optimised smoke detector layout, mechanical smoke extraction system, and visibility analysis. The CFD simulation is first validated using experimental data demonstrating a very good agreement. A case study for detector layout is then considered, showing the proposed approach increases the visibility of the egress path along the corridor of a building during fuel release and fire accident. The study will offer an effective platform for modelling fire risk and assessing the performance of fire safety mechanisms in buildings which can be also beneficial to enhance urban infrastructures safety.

- **Keywords:** Fire safety; Detector layout; Fire dynamics simulator (FDS); Visibility assessment

Li Li, Wei Gu, Bin Laiwang, Jia-Jia Jiang, Jun-Cheng Jiang, Chi-Min Shu. *Effects of 1-butyl-3-metylimidazolium tetrafluoroborate on the thermal hazard of triacetone triperoxide (TATP)*. Pages 518-525.

We investigated the thermal hazard of triacetone triperoxide (3,3,6,6,9,9-hexamethyl-1,2,4,5,7,8-hexoxonane, TATP) due to the influence of ionic liquid (IL). First, cyclic TATP was purified with a solvent mixed with methanol and 1-butyl-3-methyl-imidazolium tetrafluoroborate ([BMIM][BF4]). Second, gas chromatography/mass spectrometry (GC/MS) and Fourier transform infrared spectrometry (FTIR) were utilised to analyze the composition of the products. It was proved that the samples matched with the purchased sample to a greater extent. The thermal decomposition process of TATP was investigated by differential scanning calorimetry (DSC), thermogravimetry analyser (TGA) and vent sizing package 2 (VSP2). Based upon the data of DSC tests, the apparent activation energy (Ea) of these three samples was worked out and compared with the Starink calculation method. The maximum peak temperature (Tmax) and the average decomposition heat (ΔHd) of TATP became lower when the concentration of the [BMIM][BF4] increased because of the mixed solvent. The results of the TG experiments were consistent with those of the DSC tests. Based upon the VSP2 data, the thermal hazard data pertaining to Tmax, the maximum pressure (Pmax), self-heating rate, and the pressure rise rate were obtained. The data derived from this regard decreased when [BMIM][BF4] was added to the mixed solvent. We explored the effects of [BMIM][BF4] on the thermal decomposition hazard of TATP. The decomposition mechanism of TATP was

studied when the [BMIM][BF4] was added. Moreover, the bond dissociation energy of TATP molecule was 113.13kJ/mol calculated by Gaussian software simulation.

- **Keywords:** Ionic liquid; Thermal decomposition process; Apparent activation energy; Maximum peak temperature; Decomposition mechanism

Luis Rodríguez-Luna, Diana Bustos-Martínez, Edgar Valenzuela. *Two-step pyrolysis for waste HDPE valorization*. Pages 526-536.

Among the implemented strategies for recycling and reutilization of HDPE, pyrolysis process is considered an attractive alternative, because its potential to use waste materials to produce valuable chemical feedstock and high energy content hydrocarbons. Through pyrolysis transformation, plastics are thermally cracked in the absence of oxygen and the reaction parameters can be controlled to favor the production of specific compounds and liquid fractions. During this project, waste HDPE thermal decomposition was evaluated in a range of 450–550 °C, considering samples of 2 mm and 5 mm and a residence time of 30 min. A design of experiments was applied to find the optimal conditions to maximize the volatile fraction. Then the waste HDPE was transformed in a two-step pyrolysis in order to maximize the volatiles fraction and the intermediate and final products analyzed. According to results, A volatile fraction equivalent to the 97 % of HDPE mass was obtained at 500 °C, with a 5 mm particle size and a hold time of 30 min. The chemical analysis of wax and oil products showed that, although both blends are similarly made of alkanes, alkenes, and dienes, the compounds found in oil are shorter-chain and in a greater variety than those found in wax.

- **Keywords:** Plastic waste; HDPE; Pyrolysis; Waste to energy; Thermal degradation; Feedstock recycling

Elena Stefana, Filippo Marciano, Daniel Drolet, Thomas W. Armstrong. *A traditional Near Field-Far Field approach-based model and a spreadsheet workbook to manage Oxygen Deficiency Hazard*. Pages 537-556.

Oxygen Deficiency Hazard (ODH) poses a serious occupational risk, and represents a frequent cause of incidents, accidents, and fatalities, mostly in confined spaces and laboratories. Besides these working environments, there is a large spectrum of industries that need to manage the asphyxiation risk caused by extensive inert gas uses. In such a context, mathematical models represent a valuable tool for characterising exposure profiles under varying conditions and evaluating several exposure scenarios, prospectively or retrospectively, for new processes and/or non-routine events. To this end, the objectives of this paper are to: (1) define a traditional Near Field-Far Field (NF-FF) model to estimate the indoor oxygen (O2) concentration percent by volume and partial pressure, and (2) develop a spreadsheet workbook, called ODHMOD, for supporting occupational hygienists, safety and health practitioners, and risk assessors during ODH assessments. Both the NF-FF model and ODHMOD employ data and information usually available in companies, and predict the O2 levels time trends in working environments where inert gas releases can occur, and forced and natural ventilation can move airflows inside and/or outside. The mathematical model and its implementation in Microsoft® Excel are described, with an example of its application in a possible industrial scenario.

- **Keywords:** Exposure assessment; Two-zone; Mathematical model; Indoor air model; Inert asphyxiant gas; Occupational safety and health

Yan Cui, Jianghong Liu. *Research progress of water mist fire extinguishing technology and its application in battery fires*. Pages 559-574.

Due to its high efficiency and non-pollution, water mist fire extinguishing technology has attracted increasing interest and attention from various fire protection fields, including library fire safety, traffic hub station fire safety, ship fire safety and spacecraft fire safety. To support research and development of water mist fire extinguishing technology and its application in the field of battery fires, this paper begins by detailing the mechanisms by which water mist extinguish fires. The influence of internal and external factors on the fire suppression effectiveness of water mist is then discussed, such as water mist characteristics, additives, obstacles, ventilation conditions, fuel types and flame scales, followed by a review of researches of water mist technology in battery fires. In the final part, based on current research tendency, the paper provides future development direction and research ideas of water mist fire extinguishing technology and foresees the development prospects of its application in the battery fire field.

- **Keywords:** Water mist; Fire extinguishing mechanisms; Internal and external factors; Effectiveness; Battery fires

Tao Li, Yueping Guan, Chen Guo, Tianlei Yang, Zhenyu Yu, Guoli Xu. *Pilot scale experiment of an innovative magnetic bar magnetic separator for chromium removal from tannery wastewater*. Pages 575-580.

In this research, we designed and manufactured a pilot scale magnetic separator applying in magnetic-nanoparticles-assisted chromium containing tannery wastewater treatment. The separator is mainly composed of 186 magnetic bars and an in-situ cleaning system. The magnetic bars arranged vertically and arbitrary three magnetic bars are arranged in an equilateral triangle. Effect of dosage of magnetic particles, pH and alkali type on chromium capture efficiency and outlet chromium concentration of chromium containing tanning wastewater in laboratory scale experiments were investigated. In pilot experiment, the separator kept continuous running 15 days for 8 h per day with magnetic nanoparticles-chromium complex removed every 4 h by in-situ scraper. The treatment capacity is 16 m3/day for a device and outlet chromium concentration always less than 0.5 mg/L. The separator has simple structure and large processing capacity, and is energy-saving and easy to be scaled up. It has great potential in magnetic nanoparticles-assisted wastewater treatment.

- **Keywords:** Magnetic bar separator; Magnetic Fe3O4 nanoparticles; Tannery wastewater; Heavy metal wastewater treatment; Pilot scale experiment

Mohammad Ghorbani, Shiva Salem. *Removal of chemical oxygen demand from industrial estate sewage over hybridized anatase-graphene oxide-carbon nanotubes nanocomposite under solar irradiation*. Pages 581-590.

The aim of present work was to investigate the performance of hybridized materials, containing anatase, graphene oxide (GO), and carbon nanotubes (CNTs) in the photocatalytic treatment of sewages discharged from the industrial estate. The obtained results demonstrated the ability of hybridized nanocomposite for the solar treatment of sewages collected from different stages of industrial recovery process, between upstream of anaerobic system, and downstream of sand filter. The appropriate proportions of GO, and CNTs were determined, as 3.33 %. The effects of variables like initial COD, irradiation time, sewage collection position, and pH were evaluated on the treatment performance. If the initial COD is controlled at the level of 780 mg.l−1, the COD removal efficiency reaches to ~90 % which is the prohibitive condition in the industrial scale. The maximal photoactivity was achieved within 20 min by the control of sewage pH at the level of 8. The COD removal kinetics were related to the load of anatase nanoparticles, < 20 nm, specific surface area, 60 m2. g−1, and band gap energy, 2.1 eV, of prepared

nanocomposite which is a promising material for the wastewater cleaning in the real condition.

- **Keywords:** Industrial estate sewage; Chemical oxygen demand; Hybridized nanocomposite; Solar photoactivity; Anatase; Degradation

Zhijian Wang, Wenlei Zhao, Wenhua Du, Naipeng Li, Junyuan Wang. *Data-driven fault diagnosis method based on the conversion of erosion operation signals into images and convolutional neural network*. Pages 591-601.

In the industrial process, the safety and reliability of the mechanical system determine the quality of the product, and whether small faults can be diagnosed in time is the key to ensuring the safe operation of the system and restraining the deterioration of faults. In recent years, the data-driven fault diagnosis has attracted widespread attention in academia. However, the traditional data-driven fault diagnosis methods rely on the features extracted from expert systems, so that the effect of fault diagnosis is entirely reliant on how well the expert system can extract the features. This paper proposes a new fault diagnosis method based on AlexNet Convolutional neural network (CNN) from a data-driven perspective. Firstly, a new method for converting time-domain vibration signal into RGB image based on erosion operation (EOSTI) is proposed. Initially converted three-dimensional (3-D) images have relatively close structural elements and are difficult to identify. For such defects, the target separated RGB image is generated. Secondly, explore the classification accuracy of AlexNet to make it more suitable for fault classification of different bearing datasets. Finally, the proposed method which is tested on two datasets, including coal washing machine dataset, maintenance fault dataset, has achieved prediction accuracy of 99.43 % and 99.67 %, respectively. The results have been compared with other methods. The comparisons show the effectiveness and accuracy of the proposed approach. The result shows that this method is feasible in engineering practice.

- **Keywords:** Convolutional neural network (CNN); Fault diagnosis; Data-driven; EOSTI

Syaza I. Ahmad, Haslenda Hashim, Mimi H. Hassim, Roslina Rashid. *Inherent Safety and Economic Graphical Rating (InSafE) method for inherent safety and economic assessment*. Pages 602-609.

Incorporation of the economic aspect into the inherent safety assessment during the early design stage, especially the research and development (R&D) design stage, is currently scarce, however, there are various works which consider economic aspects at the later stage of process design. Similar economic evaluation is very hard to accomplish during the R&D design stage due to the limited amount of data available. This work introduces the Inherent Safety and Economic Graphical Rating (InSafE), a graphical inherent safety and economic evaluation for R&D design stage application. InSafE consists of gross profit and net profit margin for its economic assessment and eight inherent safety parameters taken from the GRAND method for its inherent safety assessment. Application of this method on methyl methacrylate process routes shows TBA and i-C4 routes as the safest and most profitable process routes. InSafe is also designed to be applicable for other inherent safety assessment methods for R&D design stage; for example, the Prototype Index for Inherent Safety (PIIS), the Inherent Chemical Safety Index (ICSI), and the Cumulative Index (CI). Economic evaluation during the R&D design stage enables users to compare the inherent safety level of a process route with its economic potential; hence, helping users in determining the best chemical process route in terms of inherent safety and economic potential before going to the next process design stage. If either one of these two aspects are not in accordance

with the user's preference, modifications can still be made on the process to achieve their inherent safety and economic preferences as it is still in the R&D stage of process design.

- **Keywords:** Inherent Safety Assessment; Economic Potential; Graphical; R&D Design Stage; Net Profit Margin

Chang Liu, Zhongyang Zhao, Wenchao Gao, Jakov Baleta, Wenjun Li, Qingyi Li, Minqiang Shen, Chenghang Zheng, Xiang Gao. *Process optimization of S (IV) oxidation in flue gas desulfurization scrubbers*. Pages 610-618.

At present, the control of oxidation process is imprecise in the wet flue gas desulfurization system. In this study, a modified oxidation model is established to investigate convective mass transfer of O2 and the oxidation of S (IV) under natural and forced oxidation conditions. By comparison, the model results are in good agreement with experimental results. Based on the motion of droplet in the scrubber and bubble in the slurry pool, natural oxidation rate is calculated to provide guidance for forced oxidation and recommended oxidation air flow rate. Droplet accelerates until it reaches terminal velocity. Mass transfer resistance mainly occurs in the liquid film. The mass transfer flux of the droplet with diameter of 1.5 mm increases continuously until it remains stable. The natural oxidation rate increases with the increasing of inlet O2 concentration while the forced oxidation rate increases with the increasing of oxidation air flow rate. Several gas flow rates are taken into consideration to obtain the optimal oxidation air flow rate, showing that smaller drop diameter has positive impact on oxidation process in flue gas desulfurization scrubbers.

- **Keywords:** SO2; Sulfite oxidation; Mass transfer; Scrubber

Hongchao Cheng, Yiqi Liu, Daoping Huang, Baoping Cai, Qilin Wang. *Rebooting kernel CCA method for nonlinear quality-relevant fault detection in process industries*. Pages 619-630.

Process monitoring is essential and important strategy for ensuring process safety and product quality. However, due to the nonlinear characteristics and multiple working conditions in process industries, the traditional process monitoring method cannot be effectively applied. Therefore, we propose a novel process monitoring framework, termed as mixture enhanced kernel canonical correlation analysis framework (M-NAKCCA). The innovations and advantages of M-NAKCCA are as follows: 1). The traditional CCA method is re-boosted as a new method, M-NAKCCA, to better nonlinear fault detection. Also, a matter-element model (MEm) is assimilated into M-NAKCCA to make the information more refined. 2). To overcome the curse of dimensionality that usually occurs in the high-dimensional dataset, M-NAKCCA uses the Nyström approximation technology to compress the kernel matrix. Moreover, the T2 control chart is reconstructed and the corresponding control upper limit is re-configured to improve the method sensitivity and to better the fault detection performance. 3). The proposed M-NAKCCA framework is firstly used to monitor a wastewater treatment plant (WWTP) and chemical plant with diverse process behaviors. The experimental results showed that the M-NAKCCA framework achieved the best performance for both of case studies.

- **Keywords:** Kernel canonical correlation analysis; Nyström approximation; Matter-element; Fault detection; Nonlinear industrial process

Guo-Qing Shi, Guo-Qin Wang, Peng-Xiang Ding, Yan-Ming Wang. *Model and simulation analysis of fire development and gas flowing influenced by fire zone sealing in coal mine*. Pages 631-642.

Fire zone sealing is an important approach to fire extinguishment and disaster relief. The study is aimed at investigating the distributions and evolutions of temperature and CH4 concentration fields during fire zone sealing and revealing the mechanism of sealing-induced gas explosion accidents. Firstly, the models of O2 consumption, heat production and products of coal combustion were constructed based on the Arrhenius equation of chemical reaction rate, and meanwhile the mathematical models of gases and temperature field in the sealing process were established. Besides, the variations of airflow volume, temperature and CH4 and O2 concentrations during and after fire zone sealing were numerically simulated. The results show that in the sealing process, the airflow into the fire zone gradually decreases, and air begins to flow out through the air intake at the later stage. After the completion of fire zone sealing, the temperature at fire source decreases briefly, then gradually increases and finally goes down. The temperature in the whole fire zone, except the fire source, also decreases first, then rises and finally falls gradually. The sealing raises the overall CH4 concentration in the fire zone, and the CH4 concentration at the air return side is always higher than that at the air intake side. When the sealed flow field gradually recovers to a steady flow field, the CH4 concentration goes up slowly under the influence of CH4 release. The research is of great significance for grasping the development of mine fire and the evolution of flow field in the sealing process and can provide guidance for the prevention of gas explosion accidents.

- **Keywords:** Mine fire; Fire zone sealing; Mathematical model; Fire zone temperature; Gas concentration

Zengkai Liu, Qiang Ma, Baoping Cai, Yonghong Liu, Chao Zheng. *Risk assessment on deepwater drilling well control based on dynamic Bayesian network*. Pages 643-654.

Deepwater drilling involves complex operations and equipment, so it is faced with various operational challenges including well control accidents. This paper proposes a dynamic risk assessment model for evaluating the safety of deepwater drilling operations. The dynamic risk assessment process includes three key steps: constructing fault tree models to analyze risk factors leading to a blowout accident, developing dynamic Bayesian network model based on the constructed fault trees, and performing dynamic risk analysis to evaluate the safety of well control operation. The proposed model includes risk factors about kick cause, kick detection, shut-in operation and kill operation, which covers the full process of a blowout. The proposed model could analyze the risk of blowout more comprehensively and the influencing degree of these four phases could also be clarified. Besides, the modular modelling method could update the structure and parameters of the developed model easily if new factors or data are added. The results show kick cause has the greatest impact on blowout accidents, followed by shut-in operation, kill operation and kick detection. Mutual information analysis and uncertainty analysis is performed to investigate the effects of risk factors on blowout. Finally, some corresponding preventive measures for blowouts are proposed.

- **Keywords:** Deepwater well control; Blowout; Kick; Dynamic Bayesian network

Balasubramanian Karpan, Abdul Aziz Abdul Raman, Mohamed Kheireddine Taieb Aroua. *Waste-to-energy: Coal-like refuse derived fuel from hazardous waste and biomass mixture*. Pages 655-664.

This study aimed to develop Refuse Derived Fuel (RDF) with high Calorific Value (CV) from mixed hazardous wastes and biomass. The potential utilization of newly developed RDF in cement production as a fuel substitute for coal has been investigated. In this work, five types of mixed hazardous industrial wastes (rubber waste, mixed waste, paint sludge, palm oil sludge and wastewater treatment plant sludge) and three biomass types (sawdust, paddy husk and empty fruit bunch) have been used. The newly developed RDF

developed in this study has a CV of approximately 18,652 kJ/kg, and its volatile matter, fixed carbon and ash content of 32 %, 40 % and 28 %, respectively. The study is revealed that substituting 5 ton/hour of RDF in the coal only emits about 301 mg/m3 of NOx, which is within the regulatory limits in Malaysia. Besides, the emission of heavy metals, including Zinc, Arsenic, Lead, Copper, Antimony, and Chromium, was also within the regulatory limits. RDF in cement manufacturing kilns is economically and environmentally attractive, as the combustion of RDF allows for a reduction of about 2.25 kg of CO2 per kg compared to coal. In terms of the efficiency of clinker and stack gas emission values, the substitution of 15 % of RDF to the coal at a feeding rate of 5 ton per hour in cement production did not cause any processing and quality issues in the existing cement production process. The result revealed that substituting 15 % of RDF with the coal in 5000 ton/day cement plant may reduce 112.8 USD/hour in operating cost. Additionally, 140 USD/hour of net saving could be achieved by saving 2.52 ton/hour of CO2 emitted from the cement production. Overall, the results concluded that RDF is a very promising resource recovery and waste treatment option for hazardous waste management.

- **Keywords:** RDF; Carbon dioxide emission; Hazardous waste; Economic evaluation; Coal; Cement manufacturing

Cheng Zhang, Deji Jing, Chengzhi Wu, Sujing Li, Nana Cheng, Wei Li, Gang Wang, Bixin Chen, Qiaoli Wang, Jun Hu. *Integrating Chemical Mass Balance and the Community Multiscale Air Quality models for source identification and apportionment of PM2.5*. Pages 665-675.

Source apportionment offers an efficient way to identify emission sources and the contributions to air pollution. It helps to deepen our understanding of the air pollution formation process and develop productive environmental policies. Accurate PM2.5 source apportionment is more essential for small-scale local air pollution control. An integrated source apportionment approach was built by combining chemical mass balance (CMB) model and the Community Multiscale Air Quality modelling system (CMAQ) model to complement individual model and apportion PM2.5 pollution into more elaborate emission sources categories. The CMAQ source apportionment results of corresponding PM2.5 precursors were applied to assign secondary components while that of PM2.5 were applied to assign non-local sources as the basic constrains. An island city with typical secondary components in PM2.5 pollution was chosen. The results showed the dominant source impacts of non-local sources ranged from 31.07% in summer to 49.60% in winter. Compared to individual model, the integrated source apportionment approach preserved the accuracy of CMB modelling for primary sources, simultaneously apportioned the secondary components to the primary sources and abstracted non-local sources from primary sources, which acquired more elaborate results. The results further helped develop more efficient air quality control policies.

- **Keywords:** PM2.5; CMB; CMAQ; Source apportionment; Integrated model

Xiaochuan Li, Yefeng Jiang, Jianxin Zhu, Li Wang, Mingrui Zhang, Xinhao Xu, Zhenchang Fang, Yuxuan Zhuo, Xinli Zhao, Zhihao Li, Yi Cao. *Air curtain dust-collecting technology: Investigation of industrial application in tobacco factory of the air curtain dust-collecting system*. Pages 676-683.

The air curtain system can collect the dust particles from hard-to-seal sources, which proves to be a feasible method for satisfying the increasing dust prevention requirements in China. In this study, aiming at addressing the dust escape problem at the tobacco stem loading point in a tobacco factory, a rotational flow air curtain dust-collecting system with a size of 2m x 2m x 2m was used for dust collection. The dust-collecting

characteristics using the original dust suction hood and the developed air curtain dust-collecting system were analyzed and compared. Results show that the external dust concentration when the original dust suction hood operated was as high as 83.65 mg/m3, with a dust-collecting efficiency of only 16.35 %, suggesting serious dust escape; after the use of the developed air curtain dust-collecting system, the dust-collecting efficiency reached up to 86.93~94.76 % under the same operating conditions. By studying the influence of two factors, air curtain jet velocity and exhaust-to-pressure ratio, on the dust collection efficiency of the air curtain system, at an exhaust-to-pressure ratio of 0.8 and an air curtain jet velocity of 13.5 m/s, the corresponding dust-collecting efficiency reached a maximum of 94.76 %. The present test results confirmed a better application effect of the developed air curtain dust-collecting system than the original dust-collecting system at the industrial loading point. Using the developed air curtain dust-collecting system is mainly aimed at the dust source, reduce the dust in the workshop dissemination and dispersion that can lower the transmission path of COVID-19 via aerosol.

- **Keywords:** Industrial dust; Air curtain dust collection; Dust concentration; Dust-collecting efficiency; Aerosol viral transmission

Medhat Elkelawy, E.A. El Shenawy, Salma khalaf Abd Almonem, M.H. Nasef, Hitesh Panchal, Hagar Alm-Eldin Bastawissi, Kishor Kumar Sadasivuni, Akhilesh Kumar Choudhary, Deepak Sharma, Mohammad Khalid. *Experimental study on combustion, performance, and emission behaviours of diesel /WCO biodiesel/Cyclohexane blends in DI-CI engine*. Pages 684-697.

Waste cooking oil biodiesel is considered a common way to generate clean energy in all countries. It can be used efficiently, like fossil fuel quality. To overcome the problem of poor combustion, an increase in the NOx and unburned hydrocarbon emissions, liquid, or solid additives were commonly used to improve combustion and emissions properties. In this study, the Cyclohexane (C6H12) as volatile organic and the flammable liquid compound has been applied as a micro additive for B60D40 fuel blends. Its effect on diesel engine combustion, performance, and emissions has been experimentally investigated. The C6H12 added into the diesel/biodiesel blends at different concentrations of 5, 10, and 15 % by volume basis. Two values of injection pressure have tested experimentally at different Cyclohexane concentrations. The experiment activity changed the fuel injection pressure of 150 and 250 bar, respectively, while the WCOB blends of B60D35c5, B60D30c10, and B60D25c15 have been used. The obtained results have been compared with the commercial diesel#1 and B60D40 fuel blends, respectively. The measured data show that the Cyclohexane additives dramatically improve engine emissions as well as engine performance. The CO, HC, and smoke density have decreased by increasing the Cyclohexane dose as a flammable additive. The NOx emission was reduced by increasing the C6H12 due to the fast combustion process and enhancing the premixed combustion period. Moreover, the increased injection pressure from 150 bars to 250 bars reduces the engine BSFC, HC, CO, NOx, smoke density, increasing engine BTE, CO2 emissions, and exhaust gas temperature.

- **Keywords:** Biodiesel; DI-diesel engine; Nanoparticles; Engine performance; Emission characteristics; Injection pressure; Cyclohexane

Shennan Zhou, Zhongqi Wang, Qizhong Li. *A fusing NS with NN model for the consequence prediction of vapor cloud explosion*. Pages 698-710.

Vapor cloud explosions (VCEs) have been considered as a major hazard in petrochemical industry, accompanying with wide-ranging impact and huge destruction. The existing methods are incapable to make a rapid and accurate estimation when considering multi-

factor coupling effects. Therefore, this study proposed a novel methodology of fusing numerical simulation (NS) with neural network (NN) technique for the prediction of explosion consequences. First, 6 parameters of VCEs influencing overpressure are selected as variables of a database. A CFD method is employed for simulating VCEs in a chemical site, by which sufficient blast data are generated. After the architecture of a NN model is determined, data on three generic VCEs are extracted for further model training process. A progressive training method is adopted to develop a general prediction model. Furthermore, data derived from ongoing simulation results are imported into the model for its constant self-improvement. The output of the well-trained model is subsequently transformed into a probabilistic function to assess the domino effect. The integrating NS with NN approach provides an accurate and efficient way to predict the blast effects, which can support more scientific rescue decision-making. Finally, the proposed model is applied to a case study for illustration.

- **Keywords:** Neural network (NN); Numerical simulation (NS); Vapor cloud explosion (VCE); Peak pressure prediction; Domino effect assessment

Jingde Li, Qilin Li, Hong Hao, Ling Li. *Prediction of BLEVE blast loading using CFD and artificial neural network*. Pages 711-723.

Boiling Liquid Expanding Vapour Explosions (BLEVEs) are extreme explosions driven by nonlinear physical processes associated with explosively expanded vapour and flashed liquid. Blast loading generated from BLEVEs may severely harm structures and people. Prediction of such strong explosions is not currently feasible using simple tools. Physics-based Computational Fluid Dynamics (CFD) methods are commonly utilized to predict the blast loading of BLEVE by going through many empirical formulas that map input variables to the target progressively. The calculation is often time-consuming, and it is therefore impractical to apply these methods to predict explosion loads from BLEVE in normal design analysis. Thinking of the composition of empirical relations in CFD models as a complex and nonlinear function, it is necessary to find an approximation of this function that can be efficiently calculated. The Artificial Neural Network (ANN) is a data-driven computational model that is capable of approximating any functions by learning from training data. Once properly trained, ANN can produce accurate predictions even for unseen inputs. This article presents the development of an ANN model to predict blast loading of BLEVEs in an open environment. A rigorous validation process is presented for the design of ANN structure, and the selected ANN is trained using validated simulation data from CFD models. Extensive evaluation of the network predictive performance is conducted, and it shows that the developed ANN can reproduce the result of CFD models effectively and efficiently, not only on simulation data but also on real experimental data. The prediction of ANN has a percentage error around 6 % and R2 value over 0.99 with the result of CFD simulated data. It speeds up the processing time from hours to seconds and only increases the error from 26.3 %–27.6 %, compared to the CFD simulations of real experimental data. Therefore, the developed ANN model can be potentially applied in the process engineering to generate a large number of reliable data for safety and risk assessment of BLEVEs in a more efficient way.

- **Keywords:** ANN; BLEVE; Blast wave; Peak pressure; CFD; Neural networks

Magdalena Cifuentes-Cabezas, Carlos Carbonell-Alcaina, María Cinta Vincent-Vela, José Antonio Mendoza-Roca, Silvia Álvarez-Blanco. *Comparison of different ultrafiltration membranes as first step for the recovery of phenolic compounds from olive-oil washing wastewater*. Pages 724-734.

The production of olive oil generates wastewater with a high organic load and toxicity due to the high concentration of phenolic compounds. In recent years, the study on the

treatments of these waters has been intensified together with the search for a process to recover these phenolic compounds due to their great antioxidant potential. All this with the aim of implementing the concept of circular economy. In this study, four different organic ultrafiltration membranes were evaluated in order to recover the phenolic compounds present in olive oil washing wastewater (OOWW) from an oil mill in the Valencian Community (Spain). The tested membranes differ in materials and molecular weight cut-off (MWCO): two permanently hydrophilic polyethersulfone (PESH) membranes with MWCO of 4 and 50 kDa, respectively, one polyethersulfone (PES) membrane with a MWCO of 5 kDa and a regenerated cellulose acetate (RCA) membrane with a MWCO of 10 kDa. Transmembrane pressure (TMP) and crossflow velocity (CFV) were varied from 1 to 3 bar and from 1.5 to 3.4 m·s−1, respectively. The effectiveness of the different membranes and operating conditions were evaluated comparing the permeate flux and the rejection of chemical oxygen demand (COD) and total phenolic compounds (TPhs). The membranes with lower MWCO showed stable permeate fluxes without significant changes over time, while the 50 kDa membrane showed a gradual decrease, without achieving a stable flux. Low rejection of phenolic compounds was observed in all cases, while the rejection of COD varied between 19.5 % and 62.9 % depending on the membrane and operating conditions tested. Except for the 50 kDa PESH membrane, initial permeability recovery greater than 95 % was achieved with a 35 °C water rinse, indicating that membrane fouling was not severe. Since the aim was to recover the TPhs in the permeate stream and separate them from the organic matter, the 5 kDa PES membrane at 2 bar and 2.5 m·s−1 was considered to be the best option. At those conditions a stable permeate flux of 40 L·h−1·m−2 was obtained, while the lowest TPhs rejection was observed (8.01 %) with a high COD rejection (61.18 %).

- **Keywords:** Olive oil washing wastewater; Phenolic compounds; Separation; Ultrafiltration

Tommaso Iannaccone, Giordano Emrys Scarponi, Gabriele Landucci, Valerio Cozzani. *Numerical simulation of LNG tanks exposed to fire*. Pages 735-749.

The increasing use of Liquefied Natural Gas (LNG) as a fuel for ships and vehicles poses relevant safety concerns, extended to the entire LNG supply chain and distribution network. Understanding the phenomena associated with the behavior of LNG tanks exposed to severe heat sources is thus a fundamental issue to identify potential safety-critical scenarios. The experimental data and modeling approaches currently available, mainly referring to small-scale pilot vessels, feature relevant limitations when extended to large-scale applications. In the present study, a two-dimensional non-equilibrium computational fluid dynamics model (2D CFD) of LNG tanks exposed to fire engulfing scenarios was developed. The 2D CFD model was validated against experimental bonfire data and was extended to simulate the behavior of large-scale vessels used in specific industrial applications, as the road transportation of LNG and the fuel supply of ships. A set of Key Performance Indicators (KPIs) was defined to support the safety assessment of LNG tanks, and to identify the potential transition to safety critical regions during fire exposure. The CFD results obtained allowed investigating the influence of operative parameters and geometry on the pressure build-up in the tanks, as well as on the transient evolution of complicating phenomena, such as the thermal stratification. The KPIs defined provide a useful support for the design of safety systems and for decision making in emergency response.

- **Keywords:** CFD modelling; LNG; Cryogenic tanks; Pressurization rate; Temperature stratification; Safety assessment; Emergency response

Chizubem Benson, Christos D. Argyropoulos, Christos Dimopoulos, Cleo Varianou Mikellidou, Georgios Boustras. *Safety and risk analysis in*

***digitalized process operations warning of possible deviating conditions in the process environment*. Pages 750-757.**

The process industry operates in high risks and hazardous environments that impose significant risks on workers' lives, assets-loss, and operational environments. Using the digitalized method for analyzing risk in the process operations to identify and evaluate risk emanated in the working environment is considered as a possible way of providing a warning of deviating conditions in the process environment. From this research, we realized that digitalizing process operations are highly relevant to the process industry, due to challenges such as fire, explosion, and toxic release to the environment. However, the focus on risk analysis using a digitalized method is to support decision-making by assessing and analyzing the risks associated with the operation, designing a technical system, and estimating the industry's accident and possible controlling measures. This research provides a viable solution to the process industry with risk and hazard in their process environment by installing an alarm system on the processing plant, which will give early warning information of unforeseen risk. Some of the benefits of digitalized process operations are the virtually eliminating transcription risk and hazard from the operational environment, the increased copy factor of understanding between process operation and workers, as well as to provide an early warning deviation that will interrupt the operating system. This research's findings have identified a valuable process of the digitizing process industry for useful risk analysis and protection of the operational environment.

- **Keywords:** Process safety; Digitalization; Risk; Process operations; Environment

Priscilla Grace George, V.R. Renjith. *Evolution of Safety and Security Risk Assessment methodologies towards the use of Bayesian Networks in Process Industries*. Pages 758-775.

Process Industries handling, producing and storing bulk amount of hazardous materials are a major source of concern in terms of both safety and security. Safety and security cannot be viewed separately as effective implementation of security measures in the facility requires sufficient knowledge of safety concepts as well. Traditionally, risk assessments focused primarily on accidents. The outlook towards security aspects of industries underwent a drastic change after the '9/11' terrorist attack, prompting serious research in security risk assessment methodologies. Conventional quantitative risk assessment techniques are limited due to their static nature and inability to incorporate new information and changing conditions which are characteristic of a dynamic environment. Bayesian Networks are now emerging as an effective tool to perform safety and security risk assessments dynamically by updating the prior failure probability values to accommodate new information. Bayesian networks possess the added advantage of ability to handle multi-state variables and capability to represent the conditional dependence between events. This paper provides a review of evolution of safety risk assessment and security risk assessment methodologies towards Bayesian Networks and its applications in process industries. International journal papers in the related field, published between the period 2000 and 2019 were reviewed and categorized. The intention of this review is to bring out the strengths and weaknesses of Bayesian networks as opposed to traditional and competing methods and to provide directions for future research.

- **Keywords:** Bayesian networks; Safety; Security; Dynamic risk assessment; Process industries

Mohsen Sheydaei, Baharak Ayoubi-Feiz, Ghazale Abbaszade-Fakhri. *A visible-light active g-C3N4/Ce–ZnO/Ti nanocomposite for efficient*

***photoelectrocatalytic pharmaceutical degradation: Modelling with artificial neural network*. Pages 776-785.**

Herein, a visible-light active g-C3N4/Ce–ZnO/Ti nanocomposite was successfully prepared by the immobilization of g-C3N4 and Ce–ZnO nanoparticles on a titanium grid sheet through the electrophoretic deposition method. The prepared nanocomposite was characterized by SEM, EDX, XRD, PL, photocurrent and DRS analyses. The photoelectrocatalytic activity of the catalyst was evaluated for the degradation of cefixime as a pharmaceutical pollutant. After five cycles of use, almost no weight loss of the immobilized particles was observed. The effect of operating variables i.e. catalyst dosage, solution pH, bias potential, electrolyte concentration, pollutant initial concentration and light power was investigated on the removal efficiency of the cefixime. It was observed that almost 80 % degradation was achieved at the conditions of pH 7, bias potential 0.9 V, Na2SO4 concentration 35 mM, initial cefixime concentration 10 mg/L and light power 72 W using two g-C3N4/Ce-ZnO/Ti under the visible light irradiation for 180 min. Moreover, the proposed model based on the artificial neural network could predict the photoelectrocatalytic degradation process. Sorption, electrosorption and photocatalytic processes respectively with cefixime removal efficiency of 6.7 %, 16 % and 28.7 % could not compete with the photoelectrocatalytic process. Finally, the result of TOC analysis (96 % reduction after 330 min) confirmed that g-C3N4/Ce–ZnO/Ti through the visible light photoelectrocatalytic process could effectively mineralize cefixime from aqueous solution. In addition, GC–MS analysis was employed to identify cefixime degradation products.

- **Keywords:** g-C3N4; ZnO nanoparticles; Photoelectrocatalysis; Pharmaceutical; Artificial neural network

Miljana Radović Vučić, Rada Baošić, Jelena Mitrović, Milica Petrović, Nena Velinov, Miloš Kostić, Aleksandar Bojić. *Comparison of the advanced oxidation processes in the degradation of pharmaceuticals and pesticides in simulated urban wastewater: Principal component analysis and energy requirements*. Pages 786-793.

Pollutants such as pharmaceutical products and pesticides are still present in treated water. Several of these compounds are photoactive. The photodegradation of eight organic pollutants was studied using listed advanced oxidation processes: UV/H2O2, UV/persulfate, Fenton, photo-Fenton and UV/TiO2. The results show that photodegradation is most effective in the first 10 min of treatments in simulated urban wastewater collected from the local Nišava River. To identify the correlation between applied degradation processes as well as the relationship among the structure of investigated compounds and efficiency of degradation, Pearson's correlation coefficient analysis and principal component analysis (PCA) were performed. The established correlations between the applied processes, as well as the determination of the influence of the structure on the efficiency of degradation, enable a more efficient choice of the degradation procedure, especially in the case of interference. Additionally, process electrical energy consumption and treatment costs for simulated urban wastewater with different pharmaceuticals and pesticides were determined.

- **Keywords:** UV photolysis; Hydroxyl radical; Sulfate radical; Water treatment; Pearson's correlation coefficient; Electrical energy per order

Andres Gonzalez-Cortes, Damien Burlet-Vienney, Yuvin Chinniah. *Inherently safer design: An accident prevention perspective on reported confined space fatalities in Quebec*. Pages 794-816.

The design of most industrial facilities incorporates confined spaces. Although they are not designed for human occupation, many workers penetrate them to perform tasks such as repairs, cleaning, and inspections while facing the risks of asphyxiation, drowning, and toxicity from chemical exposure. Legislative and normative frameworks recommend adopting Inherently Safer Design (ISD) principles as the primary accident prevention strategy However, confined space fatalities occur mainly during improvised interventions, emphasizing the need for designers to consider these accidents' underlying factors in their future or present projects. This paper provides an applied perspective, suggesting how practitioners can employ ISD principles to effectively overcome the inherent design deficiencies and hazards associated with confined space fatalities. For this purpose, ten confined space fatalities in six different sectors of activity were analyzed using the Causal Tree Method (CTM). Industrial process cases are included. Our results show that alternative safer designs of confined spaces or permanent adapted equipment could eliminate the need for a confined space entry or confined space work. A first model of a design-oriented solutions knowledge base, called Confined Space Permanent Collective Principles (CSPCP), is proposed. This model provides stakeholders from across various industries with an overview of safety measures that can be integrated at different life cycle phases to address confined space hazards.

- **Keywords:** Confined space; Risk reduction; Inherently safer design; Causal tree method; Accident prevention; Occupational health and safety

Xiaoxue Guo, Jie Ji, Faisal Khan, Long Ding, Yaqi Yang. *Fuzzy Bayesian network based on an improved similarity aggregation method for risk assessment of storage tank accident*. Pages 817-830.

Fuzzy Bayesian network (FBN) has been widely used for risk assessment of accidents in process industries to deal with complex causality and uncertainty arising from complex interdependence among risk factors, insufficient data and complex environments. The similarity aggregation method (SAM) is a method of aggregating fuzzy opinions considering consensus degree. However, SAM does not take into account the impact of individual differences on consistency, which will bring a certain degree of uncertainty. Therefore, this work proposes an improved SAM based FBN model to better deal with various types of uncertainty. This methodology makes the prediction results of the storage tank accident more accurate and reliable. The result analysis indicates that the improved SAM is of significance to improve the reliability of the input data of FBN. Then, the critical analysis of the root node shows the effectiveness and reliability of FBN in identifying the critical events of the storage tank accident. The proposed method can predict the probability of storage tank accidents, determine the proportion of main contributing factors and identify the critical causes of storage tank accidents more reliably and accurately. It can provide important supporting information for decision-makers to optimize risk management strategies.

- **Keywords:** Fuzzy Bayesian network; Similarity aggregation method; Storage tank accident; Risk assessment

Xianjia Huang, He Zhu, Le He, Lan Peng, Chihonn Cheng, Wanki Chow. *Improved model for estimating sidewall effect on the fire heat release rate of horizontal cable tray*. Pages 831-838.

The occurrence rate of fire events involved with cables is high and a fire hazard analysis is needed. A cable tray may be commonly placed on a wall. The fire hazards of multiple cable trays are affected by the supporting wall to give a higher maximum heat release rate. Taking the wall constraint effect on cable burning into account, a new model for the fire heat release rate of a cable tray fire against a sidewall is developed based on small scale (cone calorimeter) measurements. The newly developed model introduces a constant m to reflect the acceleration in cable burning due to the sidewall. With a

properly chosen value of m, the results obtained using the newly developed model agree well with the experimental data. The error in the peak fire heat release rate value is considerably smaller than those of other models. This work improves the understanding of the fire risk of a cable tray with a sidewall.

- **Keywords:** Cable tray fire; Wall effect; HRR estimation; HRRPUA; Developed model

Bing Li, Enyuan Wang, Zheng Shang, Xiaofei Liu, Zhonghui Li, Baolin Li, Hao Wang, Yue Niu, Yue Song. *Optimize the early warning time of coal and gas outburst by multi-source information fusion method during the tunneling process*. Pages 839-849.

Accurate and advanced early warning of coal and gas outburst is an important means to ensure the process safety of coal mining. It is a difficult problem to realize the reliable early warning of coal and gas outburst because the cause of the complex causes and disaster-causing mechanism has not been clearly defined. At present, the traditional early warning models have some problems, such as low degree of information fusion, non-dynamic decision-making, and short early warning time. To optimize the early warning time and improve the process safety of tunneling, a new early warning model is proposed. This new model is a multi-source information fusion dynamic early warning model based on combining Autoregressive Integrated Moving Average (ARIMA) and the Transferable Belief Model (TBM). The ARIMA described the changes of different types of sensor data with spatial heterogeneity over time, and the TBM fused different types of sensor data and makes dynamic decisions to achieve early warning of Coal and gas outburst. Finally, Acoustic Emission (AE), Electromagnetic Resonance (EMR), and Gas concentration data of NO.12223 conveyor roadway of Jinjia coal mine from August 3, 2017, to August 7, 2017, were used as the experimental data set. The proposed model was applied to the NO.12223 conveyor roadway of Jinjia Coal Mine to verify the dynamic early warning for the risk of coal and gas outburst. The results showed that the gas gush out with tunneling is identified 1 and 38 min in advance. It was about 9 min earlier than the earliest response EMR signal obtained by the linear regression prediction model of a single indicator used in the original monitoring and early warning system. The research results are of practical significance to optimize the time of early warning of coal and gas outburst and improve process safety risk control in coal mine production.

- **Keywords:** Coal and gas outburst; ARIMA; Transferable belief model; Multi-source data fusion; Optimize early warning time; Process safety during tunneling

Fidel Ilizástigui Pérez. *Writing 'usable' Nuclear Power Plant (NPP) safety cases using bowtie methodology*. Pages 850-857.

Historically, the majority of Nuclear Power Plants (NPP) Safety Cases have been produced and implemented under highly prescriptive regulatory regimes, with emphasis placed on demonstrations of the robustness of the facility's design basis against a set of deterministic criteria and technical standards and rules set by the Regulatory Body. This has resulted in Safety Cases that are technically sound, but at the same time too complex and not easily accessible to and usable by persons responsible for ensuring safe operations; i.e. operations and maintenance staff who are in direct control of the plant as well as managers who are accountable for safety – the key end-users. Shortcomings regarding the 'usability' of the Safety Cases are not new and have been the subject of discussion in recent years. They are deeply rooted in the way these documents are produced and implemented. It means that in order to overcome these difficulties attention should be focused primarily on the Safety Case process, affording it the same importance that is given to the final product – the documented Safety Case. This paper explores the advantages that incorporation of the Bowtie risk management methodology into the Safety Case (production) strategy can bring to the delivery of a fit-for-purpose,

accessible and usable Safety Case, supporting current efforts undertaken by the nuclear industry to ensure 'Right First Time Safety Cases'. The paper also suggests that the conduct of Bowtie workshops - in the author's opinion, the most important part of the Bowtie building process – provides vital input from the people who have most knowledge and experience of the plant and its current operational status. It enables the Bowtie diagrams to reflect the 'operational reality' in the plant, by providing a real picture of the actual barrier condition and, more importantly, to identify those barriers that need to be strengthened. The latter will have a direct effect on the usability of the resultant Safety Case product during plant operation. A generic Advanced Boiling Water Reactor (ABWR) design has been taken as an example to highlight the claimed advantages. The paper reflects how Bowtie diagrams can be built within a workshop setting that depicts how a particular accident scenario can be managed through appropriate barriers and controls. It also shows how the use of Bowtie diagrams can make the Safety Case process a true 'aid' to thinking and deliver a final product that is accessible and easy-to-understand by key end-users.

- **Keywords:** Nuclear safety cases; Safety case process; Bowtie

Boxian Chen, Suping Yu, Xuan Zhao. *The influence of RO membrane surface properties on surfactant fouling in radioactive wastewater treatment*. Pages 858-865.

Reverse osmosis (RO) has been shown to be an efficient treatment method for radioactive wastewater, which has been employed in nuclear power plants. However, the fouling on RO membrane surface should be solved to fabricate modified RO membranes with selective and fouling-resistant surface, which is essential for the further widespread application of RO. To provide fundamental insights into fouling control methods, the influence of surface properties on surfactant fouling was investigated with modified RO membranes. The results showed that surfactant fouling reduced the flux of RO membranes by 35 %–75 %. The interfacial free energies associated with the surfactants and RO membranes surface were calculated by XDLVO theory to explain surfactant fouling mechanisms. The interfacial free energies associated with CTAB and RO membrane surface increased from 3.18 to 41.22 and 69.62 mJ m−2 and SDBS increased from 20.21 to 34.07 and 43.97 mJ m−2, Tween 80 increased from -2.63 to 3.98 and 9.61 mJ m−2 with PEI and EPTAC grafting. The results indicated that the changes of interfacial free energies were mainly caused by the changes of membrane hydrophilicity and surface charge. Fabricating RO membrane with hydrophilic and neutrally charged surface was potential for improving all kinds of surfactants resistant capability. Besides, surfactant fouling had great influence on membrane permeability. The changes of radioactive nuclide rejections were mainly caused by the changes of membrane surface charge while the increase of boron rejection was attributed to the rise of membrane surface steric-hindrance. Therefore, the membrane hydrophilicity and surface charge should be carefully considered in radioactive wastewater containing surfactants treatment.

- **Keywords:** Radioactive wastewater; Reverse osmosis; Surface properties; Surfactant fouling

Y.Y. Li, G.Y. Zhu, B.S. Hou, Q.H. Zhang, G.A. Zhang. *A numerical model based on finite element method for predicting the corrosion of carbon steel under supercritical CO2 conditions*. Pages 866-884.

In this work, a numerical model, which involves mass transfer process, electrochemical corrosion at the steel/solution interface, homogeneous chemical reactions, evolution of FeCO3 film on the steel surface, was developed to predict the corrosion evolution of N80 carbon steel in the supercritical CO2 containing oilfield produced water. Meanwhile, the evolution of the physical parameters of the FeCO3 film, such as the film thickness and

porosity, and their influences on the corrosion process of steel are incorporated into the model. Different from the existed CO2 corrosion models, this model could not only predict the time-dependent corrosion rate, but also track the transient movement of corroding surface and depositing interface via the arbitrary Lagrangian-Eulerian technology. Through finite element calculation, the numerical results, especially the corrosion rate and FeCO3 film thickness, show a good agreement with the experimental data. This model aims to provide a deep insight into the complicated interaction between the corrosion of steel and the evolution of protective FeCO3 film under supercritical CO2 conditions.

- **Keywords:** Carbon steel; Supercritical CO2 corrosion; Numerical modelling studies; Finite element method; Prediction

Cassius R.N. Ferreira, Luciano R. Infiesta, Vitor A.L. Monteiro, Maria Clara V.M. Starling, Washington M. da Silva Júnior, Valério L. Borges, Solidônio R. Carvalho, Alam G. Trovó. *Gasification of municipal refuse-derived fuel as an alternative to waste disposal: Process efficiency and thermochemical analysis*. Pages 885-893.

This is the first study to investigate the use of municipal refuse-derived fuel for gasification in pilot plant scale aiming at urban waste treatment and energy generation. Energy and mass balances were applied to the thermochemical reactor based on the experimental data obtained during pilot scale operation to calculate thermal efficiency associated to the process. Volumetric composition, lower heating value, and density of the resulting syngas were determined using calorimetric tests and chromatographic analyses. The pilot plant gasification system processed 7.1 tonnes day−1 of municipal refuse-derived fuel producing 16.9 tonnes day−1 of syngas with a lower heating value of 4.6 MJ kg−1, along with 26 wt.% ash. No tar was generated during the process. According to results of this study, the pilot plant is able to generate sufficient electricity for nearly 800 small houses if connected to a steam power cycle. Pollutants emitted from syngas combustion (performed by accredited agencies) were analyzed and levels were below legal standards established in Brazil and in the United States, thus demonstrating the feasibility of this technology for conversion of municipal solid waste into a renewable energy source.

- **Keywords:** Lower heating value; Syngas; Electrical energy; Emission; Thermal energy; Waste-to-energy

Nauman Aziz, Shujaat Ali Khan Tanoli, Faiza Nawaz. *A programmable logic controller based remote pipeline monitoring system*. Pages 894-904.

Pipelines are vital method for long distance transportation and they need to satisfy levels of safety, unwavering quality and efficiency. Large amount of natural resources is wasted due to leakages in pipelines. In recent years, this issue has gained a lot of consideration in research community due to associated economic losses and environmental hazards. The precise effort of this research is to design a novel leak detection system with improved sensitivity, reduce false alarm rate and higher leak localization accuracy. The proposed test bed is established by using specific purpose sensors, A programmable logic controller (PLC) and supervisory control and data acquisition (SCADA). The well-known Volume Based Method (VBM) and Pressure Point Analysis (PPA)approach has been adapted to propose a Leak Detection System (LSD), with improved detection sensitivity and reliability. The algorithms are deployed in field on pipeline test bed and performance results are documented for different testing scenarios. Results show that the hybrid technique has leak detection sensitivity of 5 L/min in real time and ±8.5% leak localization accuracy.

- **Keywords:** Pipeline monitoring; Leak detection sensitivity; False alarm rate; Leak localization accuracy; PLC and SCADA

Jiashuo Wang, Hong Li, Xingang Li, Haifeng Cong, Xin Gao. *An intensification of mass transfer process for gas-liquid counter-current flow in a novel microchannel with limited path for CO2 capture*. Pages 905-914.

Microchemical technology shows prospect in the process intensification field of carbon capture and storage, however, there remain great challenges in microchemical technology for gas-liquid mass transfer with counter-current flow. In this work, we proposed a micro-apparatus with confined structure for gas-liquid counter-current flow mass transfer. The flow patterns on the confined structure, steady flow and bead flow, were observed, furthermore, the critical flow rate between them was measured. The influences of confined structure geometry, surface tension and viscosity of liquid on the meniscus at the gas-liquid interface were studied. The operation window of micro-apparatus with different types of confined structures was examined. The liquid loading and gas loading of micro-apparatus with S1005 were tested to be 230 μL/min and 500 mL/min, respectively. The system of absorption of pure CO2 in a 1 M NaOH solution was used to study the mass transfer. The average liquid side mass transfer coefficient of 25.1 × 10−5 m/s was measured at liquid flow rate of 30 μL/min and gas flow rate of 300 μL/min, which proves that the micro-apparatus achieves the process intensification of CO2 absorption.

- **Keywords:** Process intensification; Micro-channel; Mass transfer; Counter-current flow; CO2 capture

Lizhe Ma, Zhou Yang, Bang Ji, Yunfeng Liu, Yinlong Jiang, Jieli Duan, Wenfeng Zhao. *Comparative analysis of conventional light source and LED array combined with the catalyst for degradation of antibiotics*. Pages 915-926.

In this study, the LED array system (UV and visible light) was established, and the theoretical light distribution of the reactor was simulated in MATLAB. The light field of the conventional light source is more uniform than that of the LED array, and the light field uniformity of the LED array can optimize by increasing the number of LED. Various combinations of light sources and catalysts were subjected to batch experiments in laboratory-scale reactors. All experiments are consistent with the Langmuir-Hinshelwood model, where k UV-LEDs array [P25-Sulfamethazine]=0.0018 min−1 and k Blue-LEDs array [Ag3PO4-Tetracycline]=0.0077 min−1. In comparison experiments, conventional light sources exhibited faster dynamics compared to LED array light sources, where k Mercury lamp [P25- Sulfamethazine]=0.0209 min−1 and k Xenon lamp [Ag3PO4-Tetracycline]=0.0221 min−1. Besides, all experiments are analyzed for electric energy per order (EEO). Specifically, the EEO value of the xenon lamp is 121 times that of the blue- LEDs array when the tetracycline concentration is 50 mg/L. The UV–vis of the catalyst is also coupled with the emission spectrum of the light source to evaluate the figures-of-merit of the system. The figures-of-merit ratio of the mercury lamp to the UV-LEDs array is 58.4, and the figures-of-merit ratio of the xenon lamp to the blue-LEDs array is 69.8. The obtained model can be applied to different reactors. This work demonstrates that the photocatalytic system driven by the LED array is superior to the conventional light source system regarding photon utilization rate and sustainability.

- **Keywords:** Conventional light source; LED array; Light distribution; Photon utilization rate; Antibiotic; Photocatalytic

Didem Guleryuz. Forecasting outbreak of COVID-19 in Turkey; Comparison of Box–Jenkins. *Brown's exponential smoothing and long short-term memory models*. Pages 927-935.

The new coronavirus disease (COVID-19), which first appeared in China in December 2019, has pervaded throughout the world. Because the epidemic started later in Turkey than other European countries, it has the least number of deaths according to the current data. Outbreak management in COVID-19 is of great importance for public safety and public health. For this reason, prediction models can decide the precautionary warning to control the spread of the disease. Therefore, this study aims to develop a forecasting model, considering statistical data for Turkey. Box-Jenkins Methods (ARIMA), Brown's Exponential Smoothing model and RNN-LSTM are employed. ARIMA was selected with the lowest AIC values (12.0342, -2.51411, 12.0253, 3.67729, -4.24405, and 3.66077) as the best fit for the number of total case, the growth rate of total cases, the number of new cases, the number of total death, the growth rate of total deaths and the number of new deaths, respectively. The forecast values of the number of each indicator are stable over time. In the near future, it will not show an increasing trend in the number of cases for Turkey. In addition, the pandemic will become a steady state and an increase in mortality rates will not be expected between 17–31 May. ARIMA models can be used in fresh outbreak situations to ensure health and safety. It is vital to make quick and accurate decisions on the precautions for epidemic preparedness and management, so corrective and preventive actions can be updated considering obtained values.

- **Keywords:** Box-Jenkins method; Brown's exponential smoothing model; LSTM; COVID-19 forecasting

Wenwen Gong, Holly Barrett, Yongxia Hu, Jiajun Han, Fang Wang, Wei Wang, Shuangxi Zhou, Han Qu. *Application of biochar: An approach to attenuate the pollution of the chiral pesticide fipronil and its metabolites in leachate from activated sludge*. Pages 936-945.

The present study investigated the bio-effects and fate of the chiral pesticide fipronil and its three primary metabolites, fipronil desulfinyl, fipronil sulfide and fipronil sulfone on Chlorella pyrenoidosa and Danio rerio in the absence and presence of biochar. The results revealed that fipronil and its metabolites exhibited high toxicity to algae and fish. Enantioselectivity was observed with regard to the toxicity and degradation of fipronil and its metabolites. For Chlorella pyrenoidosa, R-fipronil was more toxic than S-fipronil and degraded preferentially during the toxicity and degradation experiments. For Danio rerio, S-fipronil exhibited higher toxicity than R- and rac-fipronil. The toxicities of fipronil sulfide and sulfone were 3–6 and 5–6 times higher, respectively, than that of rac-fipronil, and the metabolites also exhibited longer persistence. The remediation capacity for water and leachate contaminated by fipronil with the application of biochar was investigated. Biochar significantly mitigated the toxicity of fipronil and its metabolites to nontarget organisms, and reduced residues by 90 % for fipronil, 72 % for sulfone, 65 % for sulfide and 60 % for desulfinyl, whereas mitigation of only 30 %-51 % was observed in the absence of biochar. This study demonstrates that biochar has strong potential as an ideal material for the removal of fipronil and its metabolites from contaminated aquatic environments.

- **Keywords:** Fipronil; Metabolites; Enantioselectivity; Toxicity; Degradation; Remediation

Moshood Onifade. *Towards an emergency preparedness for self-rescue from underground coal mines*. Pages 946-957.

An underground mine is a workplace that is potentially unsafe. In an underground mine, when something goes wrong, seconds count and the initial reaction may be crucial to the outcome. The safety of mine workers depends on several interrelated variables such as knowledge of the dynamic, ever-changing environment, the ability to identify and respond to hazards, training, experience and communication. These factors may be critical to the response during an emergency. Mine emergencies such as fires, explosions and inundations of gas or water require immediate action and effective emergency operations management. During a mine emergency, responsible persons (and those who are trained to become responsible persons) should know how to conduct and assign a number of duties. Planning and training for such emergencies are key elements needed to increase the probability of survival. This paper provides an overview on the identification of safety practices, mine rescue teams and their tasks, safety management, etc. and shows that preparedness for self-rescue is one of the most important elements of an organized and timely emergency response to mines.

- **Keywords:** Underground coal mines; Preparedness; Self-rescue/escape; Miners; Responsible person

M.S. Romero-Güiza, J. Palatsi, X. Tomas, P. Icaran, F. Rogalla, V.M. Monsalvo. *Anaerobic co-digestion of alkaline pre-treated grease trap waste: Laboratory-scale research to full-scale implementation*. Pages 958-966.

Anaerobic co-digestion (AcoD) of grease trap waste (GTW) and sewage sludge (SS) is an attractive management option for GTW valorisation and the transition to energy-neutral wastewater treatment plants (WWTPs). The main constraints that limit the direct use of GTW as a co-substrate in WWTP anaerobic digesters are the high content of non-disabled materials (floating plastics and fibres) and the low anaerobic biodegradability rates. This study assessed a single-step alkali and sieving pre-treatment of GTW at a low temperature (<25 °C) to improve the bioavailability of GTW and facilitate its use as a co-substrate. The experimental results showed that the alkaline pre-treatment of GTW at NaOH doses of 20–30 gNaOH·kgVS−1 allowed the recovery of approximately 55–62 % of organic matter (on a volatile solids basis) present in the GTW in the form of saponified fat and generated a small waste reject fraction. Full-scale anaerobic AcoD assays (SS and pre-treated GTW) did not show inhibitory or operational problems under the experimental conditions and tested concentrations. Finally, a preliminary economic assessment for a 160 000 population equivalent WWTP in a European scenario presented a payback period of 1.75 y.

- **Keywords:** Anaerobic digestion; Co-digestion; Grease trap waste; Sewage sludge; Wastewater treatment plant

Saumitra Mishra, Kirti Bhushan Mishra. *Numerical study of large-scale LNG vapour cloud explosion in an unconfined space*. Pages 967-976.

Present work aims to predict the explosion characteristics of LNG (Liquefied Natural Gas)-air clouds in a model receiving terminal. Due to the limitations in integral/phenomenological models to include the higher cloud density effects, different terrain, obstacles and wind conditions correctly, advanced 3D CFD (Computational Fluid Dynamics) based techniques are used to model different scenarios of LNG releases. Validation against the similar experiments proved the ability of CFD code to reproduce the results with reasonable accuracy. Simulations revealed that introducing atmospheric boundary layer confines the LNG cloud with a higher level of concentrated vapour densities. The predicted flame speed in LNG-air mixture is found to be almost 35 % higher than that of a corresponding LPG (Liquefied Petroleum Gas)-air mixture leading to a higher explosion overpressure. In all considered worst-cases it is found that the predicted explosion overpressure was above 3 bar and a high value of parameter DPDX

(Spatial pressure gradient) was indicating the high likelihood of occurrence of DDT (Deflagration to detonation transition). The outcome of such a detailed study on the occurrence of DDT in an LNG plant is beneficial for setting the gas detectors layout, land-use planning and mitigation measures.

- **Keywords:** LNG-air cloud; LPG-air cloud; Dispersion; Explosion; Overpressure; DDT

K. Shojae, M. Mahdavian, B. Khoshandam, Hassan Karimi-Maleh. *Improving of CI engine performance using three different types of biodiesel*. Pages 977-993.

Currently, most automotive industries use fossil fuels, like diesel fuel, which are harmful for the environment and are known as the main reason for global warming. To reduce the adverse effects of these fuels, scholars have investigated and suggested green fuels like biodiesel. However, further studies should be conducted to improve the functionality of biodiesel fuel in diesel engines. In the current study, three completely distinct biodiesel fuels (namely, B1 with 96 % lauric oil, B2 with 88 % oleic oil, and B3 with 89.5 % ricinoleic oil) were numerically evaluated to carefully investigate the effects of the number of carbon atoms, the OH bond, and viscosity on the performance of a CI engine. First, the predicted in-cylinder pressure, the rate of heat released, and NO emissions were compared to experimental results and an appropriate accord was obtained. For the mentioned biodiesels, the parameters of engine speed, injection angle, piston bowl center depth, and compression ratio were investigated by CFD code under different engine speeds. It was found that changing the piston bowl center depth (PBCD) value from 0.0042 to 0.009 m increased NO and the indicated power by 4% and 3%, respectively, for B1, B2, and B3 biofuels. In addition, when the engine was fueled by Corylus avellana biodiesel, the change in compression ratio from 16 to 24 increased peak pressure and torque by around 77 % and 17 %, respectively. The results showed that the cylinder fueled by high viscosity biodiesel has lower air-fuel mixing. A fuel that has more oxygen atoms in its chemical structure can produce higher NO emissions. Moreover, the injection angle of 150° led to increased fuel consumption rate and indicated power compared to the injection angle of 160°. It was determined that the compression ratio has significant effects on emission and combustion characteristics.

- **Keywords:** Biodiesel; Fuel properties; Injection angle; Combustion chamber; Compression ratio

Meng Qi, Yulin Liu, Robert Stephen Landon, Yi Liu, Il Moon. *Assessing and mitigating potential hazards of emerging grid-scale electrical energy storage systems*. Pages 994-1016.

Electrical energy storage (EES) systems consisting of multiple process components and containing intensive amounts of energy present inherent hazards coupled with high operational risks. Although the thermal hazards of batteries have aroused widespread attention, the safety issues of emerging large scale EES technologies persist. This study aims to begin to fill this gap by examining the hazards of typical 100 MWh or more EES systems which are used for grid applications. These systems include compressed and liquid air energy storage, CO2 energy storage, thermal storage in concentrating solar power plants, and Power-to-Gas. Hazard assessments are performed using a hybrid method to consider and evaluate the EES systems' potential hazards from three novel aspects: storage, operability, and connectivity. Results reveal that for a similar energy storage capacity, cryogenic liquid systems have the least severe accident consequences while thermal energy storage using synthetic oil exhibits the largest. Concerning the operations in many cases, extreme operating conditions, complicated heat exchanger networks involving multiple flammable working fluids, and system operation intermittency present the major challenges to the safer operation of EES systems. Lastly,

these systems themselves form one of many components of the power supply, each of which needs to accommodate fluctuations in supply and demand but also should be prevented from transmitting hazards to each other. Considering both engineering and administrative controls, this paper concludes with a discussion on the four grouped strategies from inherent to procedural for the elimination and mitigation of the identified hazards. Representative solutions and research perspectives including inherently safer design, operation uncertainty management, resilience analysis, energy barriers design, and life cycle safety assessment are suggested for the overall safety enhancement of industrial EES systems.

- **Keywords:** Electrical energy storage (EES) systems; Hazards identification and mitigation; Consequence analysis; Hazard and operability analysis; Engineering and administrative controls

Meng Lan, Yuyang Shao, Jiping Zhu, Siuming Lo, S. Thomas Ng. *A hybrid copula-fragility approach for investigating the impact of hazard dependence on a process facility's failure*. Pages 1017-1030.

Multiple disasters induced by hurricanes such as floods, strong winds, and heavy rainfall have always been a significant threat to coastal infrastructures. However, few studies have attempted to model the dependence between hazards and study its impact on multi-hazard risks—these cognitive deficiencies inevitably affect the control of risks. This paper addresses these difficulties by first using the copulas to capture the dependence between hurricane-induced floods and strong winds based on synthetic multi-hazard events. Moreover, another two types of dependence, regression-based and mutually independent, are constructed to compare the impact of different dependence behaviors on the facility's failure. Second, the frequency of concurrent events and a scenario-based fragility function are convolved to quantify the multi-hazard risk of storage tanks. Subsequently, the annualized failure risk (AFR) and the mean return period of failure (MRPF) are used as two metrics for the multi-hazard risk. The case study results demonstrate that the BB1 copula can accurately describe the change in dependence across the full range of the multivariate distribution, avoiding overestimation or underestimation of equipment failure risks. The application of risk zoning provides decision-makers with more intuitive and convenient tools for planning and layout, highlighting the practicability of the proposed multi-hazard risk assessment method.

- **Keywords:** Multi-hazard; Hurricane; Storage tanks; Copula; Fragility; Return period