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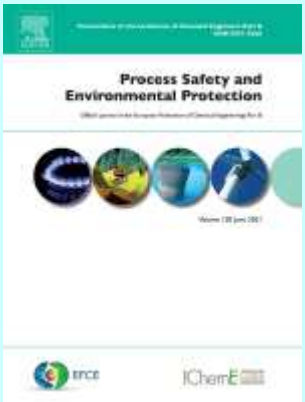

José Serrano, Nicolas Ratkovich, Felipe Muñoz, Olivier Dufaud. *Explosion severity behavior of micro/nano-sized aluminum dust in the 20L sphere: Influence of the particle size distribution (PSD) and nozzle geometry*. Pages 1-13.

Due to its industrial applications, the assessment of the explosibility parameters of aluminum powder is essential. However, they strongly depend on the Particle Size Distribution (PSD), which impacts both the rate-limiting step of the combustion mechanism and the radiative transfer. This article describes the influence of the test procedure on the explosion severity of six aluminum samples, having primary particle diameters ranging between 0.04 and 125 μm. The PSD measured in situ after dispersion in a 20 L sphere differs from those obtained before dispersion, particularly for nanoparticles for which the presence of agglomerates is evidenced. The explosion severity parameters were measured at different turbulence levels by changing the nozzle geometry and ignition delay time. The impact of the injection procedure varies from micron-sized aluminum dust to nanoparticles due to their low inertia. Moreover, if an alternative nozzle could be more appropriate at a lower turbulence level, the rebound nozzle is always the most conservative option for standard test conditions. Finally, the mean particle surface area was identified as an appropriate indicator of the micro/nano scale's explosivity performance. Results suggest that below 3 m2/g, the combustion would be diffusion-limited and kinetic-limited otherwise.

- **Keywords:** Aluminum; Dust explosion; PSD; Combustion; 20L sphere; Nozzle geometry

Maryam Azizi-Lalabadi, Meghdad Pirsaheb. *Investigation of steroid hormone residues in fish: A systematic review*. Pages 14-24.

The application of some hormones in fish production in swamps enhances fish production. However, in this regard, the critical issue is chemical contamination in water, which affects aquatic organisms. Steroid hormones (e.g., androgens and estrogens) can change the sexual characteristics of aquatic organisms, especially fish. These compounds are used in oral contraceptives and have an effect on fish at different developmental stages,

such as the development of an embryo. The residual effects of steroid hormones can adversely affect the environment, biological activities, and human health. Furthermore, these hormones negatively affect the endocrine system in marine organisms. Therefore, the identification and measure of these compounds by sensitive and selective analytical methods is not only essential, but can also prevent their adverse effects. Estrone (E1), 17β-estradiol (17β-E2), and 17α-ethynylestradiol (EE2) are current steroid hormones, which create feminized properties in male fish. The concentration of E1 in aquatic surroundings is more than the concentration of estradiol (E2) and EE2; however, E1 has a low connection and activation power to the estrogen receptor (ER). Hence, the 17β-hydroxysteroid dehydrogenases (17β-HSDs) enzyme converts E1 to E2, especially in an environment with a high E1 concentration, such as wastewater treatment. Researchers showed that E1 and its conversion have dangerous impacts on the generation and breeding of different fish species in polluted aquatic environments. In this regard, the goal of this systematic review is to evaluate the role of steroid hormones in aquatic organisms, especially fish, as well as to evaluate the negative consequences of these compounds on humans and the surrounding.

- **Keywords:** Fish; Steroid hormones; Aquatic environment; Estrone residue

Golmohammad Khoobbakht, Kamran Kheiralipour, Mahmoud Karimi. *Optimization of Chlamydomonas alga biodiesel percentage for reducing exhaust emission of diesel engine*. Pages 25-36.

One of the most important features of the biodiesel fuels to be used in diesel engines is decreasing engine emissions. In the present research, the emissions of an OM 924 Diesel Engine were modeled based on the response surface methodology under the effects of alga biodiesel as well as engine load and rotational speed to find the minimum of those amounts. The obtained quadratic models to predict the effect of input variables on the response surface were statistically significant at 1 % probability level. The amount of CO and HC emissions decreased by increasing the biodiesel percentage compared to that of pure diesel fuel. Biodiesel percentage of 65.6 and 62.6 % were the best blends in terms of minimizing CO and HC emissions, respectively. By increasing the percentage of biodiesel in the blended fuels, CO2 and NOX emissions increased and the lowest amounts of those were observed for pure diesel fuel and B6, respectively. Also, an increase in biodiesel percentage in the blended fuels caused to decrease in smoke opacity and high biodiesel percentages were the best in terms of minimizing smoke opacity. The results of multi-objective optimization showed that the lowest CO, CO2, HC, NOX, and smoke opacity emissions happened for 66.6 % biodiesel at the engine load and rotational speed of 36.9 % and 1527 RPM, respectively.

- **Keywords:** Diesel engine; Emission; Response surface method; Alga; Biodiesel

Guanyang Liu, Mason Boyd, Mengxi Yu, S. Zohra Halim, Noor Quddus. *Identifying causality and contributory factors of pipeline incidents by employing natural language processing and text mining techniques*. Pages 37-46.

The key to learning from the past incidents is to identify the underlying causes and contributory factors of the incidents. A large amount of text data on incident narratives has been accumulated over the years and can be a good learning source, if properly utilized. However, the vast amount and unstructured nature of the text data impedes generating insights on occurring patterns of incidents. This research sets upon applying natural language processing (NLP) and text mining techniques to utilize the resource for understanding contributing factors and causations behind the incidents with pipeline industry as an illustrative example. The 3587 records of incident narratives of the 'comment' section in the incident database of Pipeline and Hazardous Materials Safety

Administration (PHMSA) are exploited. Two methods of text analytics, K-means clustering and co-occurrence network, are employed to infer latent causality of incidents. The results demonstrate that both methods are capable of identifying contributing factors under specific failure types. The co-occurrence network approach exhibits advantages on extracting dependency among the contributory factors, while K-means clustering is only able to indicate general correlations. The workflow proposed in this paper provides new perspectives of identifying contributing factors and their causal dependency from incident text data for promising applications in risk analysis and accident modeling.

- **Keywords:** Incident data; Pipeline; Contributing factor; Causality; Natural language processing

Sirajum Monira, Muhammed A Bhuiyan, Nawshad Haque, Kalpit Shah, Rajeev Roychand, Faisal I Hai, Biplob Kumar Pramanik. *Understanding the fate and control of road dust-associated microplastics in stormwater*. Pages 47-57.

Microplastics (MPs) pollution in the water environment is recognized as an important environmental risk. Among the diverse sources of MPs pollution, road dust is a major contributor via stormwater runoff. Roaddust mainly originates from degradation of vehicle tyres, road marking paints, polymer-modified bitumen and the broken plastics on the surface of the road. The objective of this study is to provide a comprehensive understanding of the fate and control of MPs in the open water environment. This review critically discusses the characteristics and pathways of road dust-associated MPs in stormwater and common stormwater treatment processes used for removing MPs, and provides insight into the technical challenges of these technologies. Constructed wetland is widely used for stormwater management; however, it is found that this process is only removing 28 % MPs as they usually remain suspended or settle down very slowly in the sedimentation basin of constructed wetlands. This is because of the low density of MP particles as well as the low retention time of the wetland. Thus, untreated stormwater, rich in MPs, is released into open waterbodies. This study concludes by providing an outlook of the future opportunities of installing membrane- or flotation-based technologies in the outlet of the constructed wetland for removing 90–95 % MPs and other remaining contaminants. Such a process can produce clean water either for use in households, for sanitation, and for industrial and agricultural usage, or alternatively, for safe discharge into open waterways.

- **Keywords:** Microplastic; Road dust; Stormwater; Treatment technologies; Water environment

Chun-chen Nie, Hao Zhang, Xiao-feng Qi, Hui-yu Shang, Ting-yu Li, Peng Xue, Jun-xiang Wang, Xiang-nan Zhu. *Environment-friendly flotation technology of waste printed circuit boards assisted by pyrolysis pretreatment*. Pages 58-65.

Recycling metals from waste printed circuit boards (WPCBs) has significant economic value. Pyrolysis pretreatment was proposed to improve the flotation efficiency of WPCBs. The pyrolysis characteristics of different components were determined by thermogravimetry, which was used to determine the suitable pyrolysis temperature. Furthermore, the effects of pyrolysis on morphology, element content, phase and functional group composition of WPCBs particle were analyzed by SEM + EDS, XRD and FT-IR, respectively. Subsequently, flotation tests were carried out to determine the influence of pyrolysis on the flotation behavior of WPCBs. SEM and XRD results show that pyrolysis pretreatment has no significant effect on the surface morphology, element composition and phase composition of the WPCBs. FT-IR results indicate that pyrolysis can significantly weaken the absorption peak of organic particles due to slight

carbonization. Flotation results illustrate that the pyrolysis significantly improves the floatability of the organic components, and the float yield is increased from 6.35 % to 96.36 %. Thus, pyrolysis treatment can improve the flotation efficiency due to the greater impurity removal rate. This study provides a simple and economical pretreatment approach to enhance the flotation accuracy of different components in WPCBs.

- **Keywords:** WPCBs; Pyrolysis pretreatment; Floatability; Flotation; Metal recovery

Xianzhao Song, Jing Zhang, Dan Zhang, Lifeng Xie, Bin Li. *Dispersion and explosion characteristics of unconfined detonable aerosol and its consequence analysis to humans and buildings*. Pages 66-82.

To elucidate the dispersion and explosion characteristics of an unconfined detonable aerosol, experiments were performed with propylene oxide, JP-10 and petroleum ether. Unmanned air vehicles, a high-speed camera, infrared thermal imaging and a pressure-measurement system were used to record the experimental data. The results showed that the mean value of the fractal dimension of fuel aerosol edges decreased with increasing liquid viscosity. The initial diameter of the explosion cavity (the zone within the inner interface of the liquid shell) decreased with the increase of viscosity. An initiator charge of 500 g TNT was enough to induce a detonation in the aerosols (pure propylene oxide, 30 % petroleum ether and 70 % propylene oxide mixtures). After the aerosol was ignited, a secondary explosion phenomenon was observed and its characteristics were discussed. Furthermore, consequence analysis to determine the damage to humans and buildings were quantitatively assessed by using PROBIT equations. The relative-safety radii for humans and buildings were also obtained.

- **Keywords:** Detonable aerosol; Overpressure; Impulse; DDT; Consequence analysis

Mingrui Yang, Haipeng Jiang, Xiangfeng Chen, Wei Gao. *Characteristic evaluation of aluminum dust explosion venting with high static activation pressure*. Pages 83-96.

Aluminum dust explosion venting experiments with static activation pressure ranging from 70 kPa to 280 kPa were conducted in the 20 L spherical chamber with venting diameters from 20 mm to 125 mm. For the case of high activation pressure, the maximum flame length in experiments is 1.64 m, which is close to the prediction of standard, while the maximum width is significantly smaller than the prediction. New fitting formulas in a laboratory scale for flame length and width are obtained, which provide a reference for venting safety area design, and the effect of activation pressure, dust concentration and venting area are taken into account. By the comparison, the external pressure prediction of EN14491 shows a good performance and NFPA68 has an opposite trend with experiments. Based on the experimental results, it is found that the the external pressure attenuation is inversely proportional to the distance, which is different with the coefficient of the distance suggested by the standard EN 14491.

- **Keywords:** Dust explosion venting; Flame length; Flame width; Reduced pressure; External pressure

Daniel Ulloa-Ovares, Carlos E. Rodríguez-Rodríguez, Mario Masís-Mora, J. Esteban Durán. *Simultaneous degradation of pharmaceuticals in fixed and fluidized bed reactors using iron-modified diatomite as heterogeneous Fenton catalyst*. Pages 97-107.

The aim of this study was to evaluate the use of pelletized iron-modified diatomite as heterogeneous Fenton catalyst for the removal of carbamazepine, clindamycin,

gemfibrozil, ketoprofen, florfenicol, and sulfamethazine, and to compare its performance in fixed and fluidized bed reactor configurations. The prepared catalyst pellets were characterized by XRD, SEM, ED-XRF, BET, and compression strength analysis. Applying a Taguchi L9 design of experiments, the oxidation of a mixture of six common pharmaceuticals was studied under different operating conditions (initial pH, particle size, space time, and H2O2 initial concentration) for both reactor configurations. Under the best operating conditions, overall pharmaceutical degradations by the Fenton reaction were 32.6 % and 31.8 % in the fluidized and fixed bed reactors, respectively. Among the analyzed pharmaceuticals, clindamycin was the one presenting the highest removal (88.8 % fixed, 89.7 % fluidized), followed by gemfibrozil (70.4 % fixed, 100 % fluidized), ketoprofen (36.2 % fixed, 35.1 % fluidized), carbamazepine (19.0 % fixed, 21.1 % fluidized), sulfamethazine (18.1 % fixed, 21.1 % fluidized), and florfenicol (4.6 % fixed, 7.0 % fluidized). The initial pH was the most sensitive variable, presenting the best performance at pH 3. After 10 h of operation, the catalyst suffered a 27.9 % decrease in its activity when operated in the fixed bed reactor, whereas in the fluidized bed reactor its deactivation was 52.1 %. The catalyst was also evaluated in a real wastewater matrix, showing basically the same activity as in synthetic wastewater; TOC overall removal was 31 % for the fixed bed and 36 % for the fluidized bed reactor. Finally, the electrical energy per order (EEO) consumed in both reactors was calculated to compare their energy efficiency; the fixed bed configuration presented the lowest value (1.01 Wh/m3/order), suggesting that this is a more energy-efficient configuration for commercial wastewater treatment applications.

- **Keywords:** Fenton reaction; Catalytic systems; Emerging contaminants; Removal strategies; Heterogeneous reactor; Wastewater

Jianqi Chen, Lu Wang, Shihao Ma, Yujie Ji, Bing Liu, Yuan Huang, Jianping Li, Hualin Wang, Wenjie Lv. *Separation of fine waste catalyst particles from methanol-to-olefin quench water via swirl regenerating micro-channel separation (SRMS): A pilot-scale study*. Pages 108-116.

From the perspective of resource reserves, the development of coal-based methanol-to-olefins (MTO) technology is regarded as an important direction for the sustainable development of the chemical processing industry in China. However, the wastewater generated in the process of industrial operation has a significant impact on the stability of the process. To remove the fine waste catalyst particles from MTO quench water, a swirl regenerating micro-channel separation (SRMS) technology was developed. A 25 m3/h pilot-scale study was conducted to examine the separation and regeneration effects under different operating parameters and verify the feasibility of this technology through a long-duration experiment. Results showed that for filtration velocities ranging from 11 to 15 m/h, the total separation efficiency was 95–99 %, the removal efficiency of 0.2 μm particles was 83–90 %, and the regeneration cycle was 24–40 h while the waste catalyst particle concentration in quench water was 300–600 mg/L. The optimum regeneration water and gas speeds were determined to be 11–15 m/h and 56.6 m/h, respectively. Moreover, the performance of the pilot plant over 600 h continuous operation effect of was tested, and an average separation efficiency > 95 % with excellent regeneration was obtained.

- **Keywords:** Hydrocyclone intensified filtration; Deep bed filtration; Methanol-to-olefin; Wastewater; Fine waste catalyst

Pengbo Hu, Shujuan Wang, Yuqun Zhuo. *Research on operation parameters and properties of flue gas on adsorption of As2O3 by γ-Al2O3: An experiment and simulation study*. Pages 117-130.

How operation parameters (e.g. flow speed of flue gas and temperature) and flue gas properties (e.g. contents of SO2, NOx etc.) affect As2O3 adsorption by γ-Al2O3 under the condition of selective catalytic reduction (SCR) is the key to protecting catalyst from poisoning and preventing it being emitted into environments. The patterns of mentioned influence factors affecting adsorption of As2O3 have been investigated via experimental studies combined with molecular dynamics (MD) simulation calculations. According to the results of experiments and MD simulation, within the selected specific range of flue gas flow speed, As2O3 could be adsorbed effectively. In the meantime, with higher temperature, the thermal vibration of As2O3 molecule gets more intense and compromises the adsorption. Also, different flue gas contents affect As2O3 adsorption in different chemical and physical means. This research could provide valuable information for power plants and subsequent studies in related area.

- **Keywords:** Adsorption; As2O3; Operation parameters; Flue gas; Experiments; MD

Kuang Cheng, Xiangyu Zhao, Wang Zhou, Yi Cao, Shuang-Hua Yang, Jianmeng Chen. *Source term estimation with deficient sensors: Traceability and an equivalent source approach*. Pages 131-139.

In air pollution monitoring, source term estimation (STE) is a problem to inversely estimate the source parameters, such as their locations and emission rates, with available information of meteorology, ground geometry, as well as concentration measurements and their locations. For chemical industrial parks (CIPs), a major challenge of the estimation is the ill-posedness caused by the lack of sufficient measurements to match a vast number of undetermined source parameters. This ill-posedness results in incapacity in estimating unique solution for unknown source parameters, hence they are untraceable. In this paper, a theoretical definition of traceability is introduced to give a general criterion to determine whether a STE problem has a unique solution. This is derived from an atmospheric transport and dispersion model with description of linear sensitivity of measurements to source parameters. Based on this traceability criterion, an equivalent source method to convert an untraceable problem to traceable is proposed. The performance of this method is evaluated with a numerically simulated case whose configuration is based on information collected from a CIP in Shangyu, China. The results suggest that traceability is vital to STE problems. The method is effective for solving daily STE problems with sensor deficiency encountered in CIPs.

- **Keywords:** Source term estimation; Inverse modelling; Traceability; Air pollution; Chemical industrial park

Mohamed A. Eltawil, Hasan A. Alhashem, Abdulrahman O. Alghannam. *Design of a solar PV powered variable frequency drive for a bubbler irrigation system in palm trees fields*. Pages 140-153.

This work aims to design a standalone solar photovoltaic (SPV) system to operate variable frequency drive (VFD) for palm trees irrigation using bubblers and control the irrigation network. A complete irrigation system is designed and constructed in two fields of date palm trees. A small photovoltaic (PV) system is used to operate the rainbird controller which changed water delivery from one subline to another after a predetermined time. The performance of the developed system is evaluated under different operating factors and its costs are analyzed. Water distribution uniformity and soil moisture at different depths in the root zoon are measured. The frequency of supply voltage is influential in controlling the speed of the induction motor, whereby operating the inverter, the motor speed is constant without any oscillation. Irrigation through the last two laterals in field II indicated that the required maximum hydraulic energy and maximum PV array power was 7.81 kW h/d and 3.74 kWp, respectively at the total

dynamic head of 22.75 m. The coefficient of variation of bubblers flow was a small value for a single lateral (3.83 %), while for two laterals it varied from 8 to 12 %. The total dynamic head reached about 22.75 m for the last sublines in field II. The average subsystem efficiency was about 0.41. The annual cost of unit power of PV system was 0.161 $US /kWh without subsidies. The proposed SPV pumping is cost-effective and controlled the motor efficiently without energy backup.

- **Keywords:** Solar photovoltaic; variable frequency drive; Palm trees irrigation; Solar pumping; Bubbler; Economic

Thi Hai Nguyen, Anh Thao Nguyen, Paripurnanda Loganathan, Tien Vinh Nguyen, Saravanamuthu Vigneswaran, Thi Hoang Ha Nguyen, Hai Nguyen Tran. *Low-cost laterite-laden household filters for removing arsenic from groundwater in Vietnam and waste management*. Pages 154-163.

This study evaluated the performance of a low-cost natural laterite from Thach That (NLTT), Vietnam, for its capacity to remove arsenic (As) in a household filter with contaminated groundwater. The NLTT was initially tested in a laboratory column trial lasting 800 h. The breakthrough curves were found to fit the Thomas model very satisfactorily with adsorption capacities of 0.06 and 0.20 mg/g at a flow velocity of 0.85 m/h for the influent As(V) concentrations of 0.1 and 0.5 mg/L, respectively. In household filters at four sites, the median As concentration in groundwaters (0.04–0.19 mg/L) dropped to 0.026–0.054 mg/L after traditional sand filtration. However, following subsequent NLTT filtration through columns (14 cm inner diameter, 65 cm height) at 0.65 m/h flow velocity, it fell to below the Vietnam and WHO drinking water standard (0.01 mg/L) during seven months of continuous operation. Portland cement and lime were tested as binding agents for the exhausted NLTT waste in a solidification/stabilization process at different ratios. The best ratio of exhausted NLTT: Portland cement: lime for restraining mobility of As from this waste was 3:1:0.5. The concrete brick products exhibited a suitable compressive strength for using it as building materials in construction work.

- **Keywords:** Arsenic removal; Adsorption; Laterite; Household filter; Solidification/stabilization

Chuanyu Pan, Xishi Wang, Guochun Li, Jiangyue Zhao, Meilin Liu, Yangpeng Liu, Xiaolong Zhu. *Influences of multi vents' numbers and distributions on vented ethanol-gasoline vapor deflagrations*. Pages 164-177.

The safety issues and existing risks of ethanol-gasoline in industrial production have to be well considered and investigated. Especially when there are more than one thin doors, windows/thin walls in containers were broken once deflagrations occurred, but it appears that few researches deal with multi vented deflagrations. Hence we carried out experiments in a small cuboid container to investigate the effect of multiple vents' numbers and distributions on vented ethanol-gasoline vapor deflagrations characteristics. Multi overpressure peak structures during multi-vented deflagrations were first observed and analyzed to reveal the complex physical process in the venting. Results show that five overpressure peaks' structures were found (Pb, Pfv, Pcv, Pext and Pac) when multiple vents with the same area are arranged along the axis of the container's roof. Flame propagation and overpressure buildup are mainly influenced by the 1st vent (i.e., the nearest one to the spark plug). The 1st vent also determines the number and types of overpressure peak structures. Compared with the single vent, the cases of multiple vents with the constant total vent area may cause larger Pmax, dP/dtmax and KG even if

all vents are closer to the spark plug. Consequently, the use of multiple vents does not necessarily help to improve the vent effects.

- **Keywords:** Multiple vents; Safety design; Typical overpressure peaks; Ethanol-gasoline; Multi vented deflagration

Jasim I. Humadi, Saba A. Gheni, Safaa M.R. Ahmed, Ghassan H. Abdullah, Anh N. Phan, Adam P. Harvey. *Fast, non-extractive, and ultradeep desulfurization of diesel in an oscillatory baffled reactor*. Pages 178-187.

Sulfur compounds are major contaminants in diesel fuels and cause significant negative impacts on the environment, human health, and petroleum product quality. Oxidative desulfurization (ODS) has gained attention due to relatively mild operating conditions. However, ODS requires significant improvements in terms of productivity, reaction time, and conversion. This study reports the development of a highly efficient, rapid ODS process, in an oscillatory baffled reactor (OBR), to allow continuous, safe dibenzothiophene (DBT) removal. DBT conversion was studied as a function of temperature, residence time, oscillation frequency, and oscillation amplitude. By optimizing the operating conditions, up to 94 % DBT could be removed without further extraction in 3 min, at 80 °C, 4 Hz, and 6 mm. This is a substantial increase over comparable processes at this temperature and furthermore has been conducted in a reactor that scales up predictably, hence it is probable that this performance can be realized at an industrial scale.

- **Keywords:** Oxidative desulfurization; Oscillatory baffled reactor (OBR); Acetic acid; Hydrogen peroxide

Mehmet Kobya, Philip Isaac Omwene, Sanaz Mohammadzadeh Sarabi, Sadullah Yildirim, Zubeda Ukundimana. *Phosphorous removal from anaerobically digested municipal sludge centrate by an electrocoagulation reactor using metal (Al, Fe and Al-Fe) scrap anodes*. Pages 188-200.

Phosphates are a major cause of eutrophication and growth of algal blooms in surface waters. The current study investigated phosphorus removal from sludge centrate effluent (SCE) of a municipal wastewater plant by packed-bed electrocoagulation (EC) reactor. Distinctively, iron (Fe), aluminum (Al) and Al-Fe hybrid scrap anodes were used. The influence of initial pHi, applied current and packed anode bed density were evaluated. Phosphorous removal efficiency of 99.99 % was obtained at applied current of 0.20A with anode bed densities of 0.18 kg Al/m3 (pHi 5.0) and 0.48 kg Fe/m3(pHi 7.0). Optimum operating costs entailing sludge disposal, chemical, energy and electrode consumption were calculated as 0.379 US $/m3 (6.04 $/kg PO4-P) for Fe scrap, 0.494 US $/m3 (9.46 $/kg PO4-P) for Al scrap and 0.501 US $/m3 (9.59 $/kg PO4-P) for Al-Fe hybrid scraps. Phosphorus removal per electrochemically generated metal was 191.22 mg P/g Al, 104.88 mg P/g Fe, and 61.08 mg P/g (Al + Fe). The molar metal to phosphorus ratio at optimum conditions were calculated as 5.41, 3.97 and 7.65 mol/mole for Al, Fe and Al-Fe, respectively. The key mechanisms for phosphorus removal were metal-phosphorus precipitation and adsorption. Herein, metal scrap anodes have been proved effective for phosphorous removal from SCE.

- **Keywords:** Phosphorus; Electrocoagulation; Al and Fe scraps; Sludge centrate

Gending Yu, Yulan Wang, Liang Zheng, Jiale Huang, Jingling Li, Lingzhu Gong, Rongguo Chen, Wei Li, Jiulai Huang, Yih-Shing Duh. *Comprehensive study on the catastrophic explosion of ammonium nitrate stored in the warehouse of Beirut port*. Pages 201-219.

On August 4 in Beirut Port, Lebanon, a catastrophic explosion occurred at a warehouse, claiming 204 deaths and injured more than 7000 individuals, with a property loss of approximately US$ 15 billion. An extensive consequence analysis based on the crater size and physical effects for the estimation of the quantity of exploded ammonium nitrate was performed. By using satellite images and integration methods, the crater diameter was determined to be 112.9 m. From the scaling laws, overpressure effect on structures, and inverse analysis, the trinitrotoluene equivalent mass of exploded ammonium nitrate was approximately 950.3 tons. Based on the results of the consequence analysis performed by three methodologies, it can be concluded that the warehouse not only stored a substantially large quantity of ammonium nitrate but was also located too close to the adjacent communities and residential districts without an adequate safety distance. Judging by the simulation results of overpressures and explosive blast on structures, a fatality radius is determined to be about 487 m from the explosion center. Some more lessons related to the time to explosion, phenomena of sympathetic detonation, arrival time of blast, safety distance, fatalities/injuries versus the equivalent mass of trinitrotoluene and a maximum allowable quantity of 30 tons have been learned to be the important guides for safety measures and revisions for limiting the amount of ammonium nitrate under storage.

- **Keywords:** Beirut explosion; Major chemical accident; Ammonium nitrate; Domino effect; Sympathetic detonation

Jiri Pecha, Michaela Barinova, Karel Kolomaznik, Thanh Nhu Nguyen, Anh Tuan Dao, Van Thi Le. *Technological-economic optimization of enzymatic hydrolysis used for the processing of chrome-tanned leather waste*. Pages 220-229.

Chrome-tanned solid waste generated in large quantities by the leather industry poses a major threat not only to the environment, but also to living organisms including humans because of its potential toxicity. The crucial issue determining viable industrial processing and valorisation of this waste is the process economy. In this work, a mathematical model that enables technological simulation of complete process for chrome shavings utilization by alkali-enzymatic hydrolysis was developed and incorporated into an economic optimization model. The model includes experimentally verified quantitative description of the dependence of reaction rate on enzyme concentration, an important factor which so far has not been addressed in this context. The simulation calculation showed that the enzyme optimal concentration usually lies in a relatively narrow area between 0.2 and 0.4 % wt. of the feedstock dry matter at standard reaction conditions. Such optimization can save considerable portion of the processing costs – as much as 43 % at given calculation parameters – and improve the plant capacity and annual profit leading to the reduction of payback period from initial 4.7 years to final 1.5 year. The results obtained through this engineering approach are valuable not only for the processing plant operation, but also for the overall process design including the design of process control algorithms, and therefore are applicable and adjustable for a wide range of cases, from individual waste producers to centralized leather waste processing.

- **Keywords:** Chrome-tanned waste; Enzymatic hydrolysis; Enzyme kinetics; Techno-economic optimization; Process simulation

Xingwei Zhen, Yue Han, Yi Huang. *Optimization of preventive maintenance intervals integrating risk and cost for safety critical barriers on offshore petroleum installations*. Pages 230-239.

Preventive maintenance (PM) of safety critical barriers on offshore petroleum installations is an important activity for protecting against major offshore accidents. However, it is worth noting that the increased risk and maintenance cost during the PM task is often left

out in the determination of PM interval. In this paper, a multi-objective optimization approach is proposed with newly-defined risk, cost criteria and constraints to determine the optimum PM intervals for safety critical barriers on offshore petroleum installations. The proposed framework is comprehensive and quantitative, which comprises three main modules: initialization of PM interval set, risk assessment & maintenance cost evaluation, and multi-objective optimization with PSO. Details and the related results of the three modules are given. The case study validates the effectiveness of the proposed framework and reveals that the increased risk during the PM task has a significant impact in the determination of PM intervals. The results also demonstrate that a longer interval can be recommended when the risk increase, risk reduction and maintenance cost are taken into consideration comprehensively. The presented approach achieves the optimization of PM intervals integrating risk and cost for safety critical barriers on offshore petroleum installations, which is capable of guiding the PM implementation with higher accuracy for the offshore petroleum enterprises.

- **Keywords:** Preventive maintenance; Optimization; Interval prediction; Maintenance cost; Risk

Igor S. Anufriev, Evgeny P. Kopyev, Ivan S. Sadkin, Mariia A. Mukhina. *NOx reduction by steam injection method during liquid fuel and waste burning*. Pages 240-248.

Incineration is the most common liquid combustible waste disposal method. However, when waste is incinerated, huge amounts of toxic combustion products are formed. The use of steam in the combustion process helps to reduce the toxic emissions. In this work, the effect of steam on the flame characteristics during combustion in a laboratory burner is investigated using diesel fuel as an example. The principle of burner operation is based on liquid fuel spraying by a steam jet as efficient way of liquid combustible waste disposal with heat energy production. The steam gasification of the incomplete combustion products increases the carbon burnout degree and the steam presence in the combustion zone reduces thermal nitrogen oxides formation. Thus, two environmental problems are simultaneously solved: waste disposal and reduction of toxic products. Laboratory experiments were carried out to measure the composition of intermediate combustion products and temperature in the flame of the burner. Comparison of results obtained with steam or air supply under equal conditions showed that the CO content in the regimes with air is 25 % higher than in the regimes with steam; the content of nitrogen oxides in the regime with steam is 30 % lower than in the regime with air.

- **Keywords:** Combustion; Liquid waste disposal; NOx reduction; Superheated steam; Flame characteristics

Prasanjit Dey, S.K. Chaulya, Sanjay Kumar. *Hybrid CNN-LSTM and IoT-based coal mine hazards monitoring and prediction system*. Pages 249-263.

IoT-enabled sensor devices and machine learning methods have played an essential role in monitoring and forecasting mine hazards. In this paper, a prediction model has been proposed for improving the safety and productivity of underground coal mines using a hybrid CNN-LSTM model and IoT-enabled sensors. The hybrid CNN-LSTM model can extract spatial and temporal features from mine data and efficiently predict different mine hazards. The proposed model also improves the flexibility, scalability, and coverage area of a mine monitoring system to an underground mine's remote locations to minimize the loss of miners' lives. The proposed model efficiently predicts miner's health quality index (MHQI) for working faces and gases in goaf areas of mines. The experimental results demonstrated that the predicted mean square error of the proposed model is less than 0.0009 and 0.0025 for MHQI; 0.0011 and 0.0033 for CH4 in comparison with CNN and LSTM models, respectively. The less means square error

indicates the better prediction accuracy of the trained. Similarly, the correlation coefficient (R2) value of the proposed model is found greater than 0.005 and 0.001 for MHQI; 0.007 and 0.001 for CH4 compared to CNN and LSTM models, respectively. Thus, the proposed CNN-LSTM model performed better than the two existing models.

- **Keywords:** IoT; Deep learning; Underground coal mine; Prediction of hazards; Miner's health quality index

Wei Liu, Hao Xu, Deyao Wu, Yueping Qin, Jia Liu, Wei Zhao. *Gases migration behavior of adsorption processes in coal particles: Density gradient model and its experimental validation*. Pages 264-277.

The injection of CO2 or N2 to displace CH4 in coal seams can improve coalbed methane (CBM) recovery. However, the migration pattern of these gases in the coal matrix is disputed as the Fick diffusion model is not fully applicable. In this work, the isothermal adsorption experiments of CO2, CH4 and N2 were first performed on four kinds of coal samples. A mathematical model of gas diffusive adsorption was then established based on a free gas density gradient (FGDG) drive, which was solved numerically by finite difference method (FDM). The microchannel diffusion coefficient (Dfg) that reflected the transport capacity of free gas in the coal matrix was determined through matching the simulation curves of cumulative gas adsorption with experimental data. Furthermore, the effects of gas type, coal rank and adsorption pressure on the microchannel diffusion coefficient were quantitatively investigated. The results show that (i) the simulation results of the gases are well consistent with the experimental data, indicating that the migration behavior of CO2, CH4 and N2 in coal particles conforms to the FGDG-driven model; (ii) the Dfg of CO2 is much higher than that of CH4 and N2, and the Dfg of a single gas shows an asymmetric U-shaped trend with the coal rank; (iii) compared with Fick's diffusion coefficient and Darcy's permeability coefficient, the Dfg is only related to the pore structure of the coal and gas properties, independent of the state parameters such as pressure and time. Therefore, the FGDG-driven model better explains the essence of gases migration behavior in the coal particles, and this model can be considered as an important aspect of CBM production calculation and prediction.

- **Keywords:** Coalbed methane; Coal particles; Gas adsorption and migration; Free gas density gradient; Mathematical modeling

Baoquan Xin, Wenyi Dang, Xingqing Yan, Jianliang Yu, Yongzhong Bai. *Dispersion characteristics and hazard area prediction of mixed natural gas based on wind tunnel experiments and risk theory*. Pages 278-290.

As a complex mixture, high-hydrogen-sulfide natural gas has a high risk of poisoning and explosions after leakage. This study combined wind tunnel experiments, computational fluid dynamics (CFD) technology, and risk theory to explore the dispersion characteristics and hazardous area of released mixed natural gas (M-NG) in complex terrain. Based on risk theory, various external safety protection distances under four kinds of risk criteria were predicted. The results indicated that the dispersion process of M-NG in mountainous terrain can be divided into two components: downhill dispersion and cut-slope dispersion. At the same wind speed, the maximum concentrations for different wind directions can differ by a factor of 10. Compared with the results of the wind tunnel tests, the maximum overestimation was 62.9% when simulating the near-field dispersion of M-NG by CFD, while the underestimation was 28.1% for the far-field dispersion. The critical distance was about 1042 m, the dispersion time was 960 s, and the gas concentration was 42 ppm. The wind speed, wind direction, topography, and their interactions have an important impact on the dispersion process and hazard area of M-NG. The study also indicated that in the quantitative risk assessment, more attention should be paid to the toxic hazard of hydrogen sulfide in M-NG rather than the explosion hazard caused by methane. The risk method fully considers the frequency of accidents and the types of

protection targets. It can thus be used as a reference for site selection, land use planning, and emergency protection.

- **Keywords:** Wind tunnel experiment; Gas dispersion; Mixed natural gas; Hydrogen sulfide; Quantitative risk assessment; Emergency protection

Biao Jin, Jianwan Ji, Wuheng Yang, Zhiqiang Yao, Dandan Huang, Chao Xu. *Analysis on the spatio-temporal characteristics of COVID-19 in mainland China*. Pages 291-303.

COVID-19 has brought many unfavorable effects on humankind and taken away many lives. Only by understanding it more profoundly and comprehensively can it be soundly defeated. This paper is dedicated to studying the spatial-temporal characteristics of the epidemic development at the provincial-level in mainland China and the civic-level in Hubei Province. Moreover, a correlation analysis on the possible factors that cause the spatial differences in the epidemic's degree is conducted. After completing these works, three different methods are adopted to fit the daily-change tendencies of the number of confirmed cases in mainland China and Hubei Province. The three methods are the Logical Growth Model (LGM), Polynomial fitting, and Fully Connected Neural Network (FCNN). The analysis results on the spatial-temporal differences and their influencing factors show that: (1) The Chinese government has contained the domestic epidemic in early March 2020, indicating that the number of newly diagnosed cases has almost zero increase since then. (2) Throughout the entire mainland of China, effective manual intervention measures such as community isolation and urban isolation have significantly weakened the influence of the subconscious factors that may impact the spatial differences of the epidemic. (3) The classification results based on the number of confirmed cases also prove the effectiveness of the isolation measures adopted by the governments at all levels in China from another aspect. It is reflected in the small monthly grade changes (even no change) in the provinces of mainland China and the cities in Hubei Province during the study period. Based on the experimental results of curve-fitting and considering the time cost and goodness of fit comprehensively, the Polynomial(Degree=18) model is recommended in this paper for fitting the daily-change tendency of the number of confirmed cases.

- **Keywords:** COVID-19; Spatial-temporal characteristics; Impact indicators; Correlation analysis; Curve-fitting

Xiaojiao Cai, Wen Nie, Shuai Yin, Qiang Liu, Yun Hua, Lidian Guo, Lei Cheng, Qingxin Ma. *An assessment of the dust suppression performance of a hybrid ventilation system during the tunnel excavation process: Numerical simulation*. Pages 304-317.

The high concentration of dust particles produced during excavation processes in mine tunnels are a serious threat to workers' health. Accordingly, in order to ensure safe production in mines, it is of vital importance to gaining an in-depth understanding of the dust pollution control rules in a tunnel. The appropriate use of far-pressure-near-absorption (FPNA) ventilation systems can contribute to achieving the suppression of dust in a working face and safeguarding workers' health. In this study, through the use of computational fluid dynamics' (CFD) techniques, numerical simulations were performed in a tunnel to assess the dust suppression performance of a hybrid ventilation system. In these simulations, the air exhaust quantity (Qc) and the height of the air pressure duct above the tunnel floor (Dy) were set at different values. The simulation results were validated using data from field measurements. If the pressure air quantity (Qy) remained unchanged the diffusion distance of highly concentrated dust decreased with an increasing Qc. From an economic perspective, 550 m3/min was determined to be the optimal value for Qc. When Qc was fixed at 550 m3/min but Dy was increased, the

diffusion distance of highly concentrated dust first decreased and then increased. Therefore, an optimal dust suppression performance was achieved when Qc = 550m3/min and Dy = 2 m. The present study therefore provides a new scheme for improving the underground operating environment and achieving safer production.

- **Keywords:** Tunnel excavation; Far-pressure-near-absorption (FPNA) system; Dust suppression performance; Numerical simulation

Yu Wang, Xuning Zhuang, Fei Li, Xiaolong Song, Weihua Gu, Jianfeng Bai, Ruixue Wang. *Effects of polarizer on the metals migration and transformation behaviors during the thermal treatment of discarded LCD panels*. Pages 318-326.

Thermal treatment has been proved as an efficient and promising method for LCD panel scraps pre-treatment and resource recycling. However, undesirable pollutants including polycyclic aromatic hydrocarbons (PAHs) and heavy metals tend to occur during the thermal treatment. To better understand the metals migration behavior and to illustrate the interaction effect between organics and metals, effect of the polarizer on the metals (Cr, In, Ni, Cu, Zn, Fe) migration and transformation behaviors was analyzed in this study. Results showed that polarizer, the main organic component in LCD panel, could enhance the metals migration behavior during the thermal treatment and also affect the metals speciation distribution in solid residue. The enhancement effect on metals migration rate was mainly deduced by the gas/volatile compounds from polarizer decomposition, while the metals speciation distribution in solid residue was mainly affected by the solid product from polarizer decomposition. The polarizer also showed increase effect on the potential risk of In, Cu and decrease effect on Fe in solid residue. The results suggest that reducing the organics content or adding solid carbon in treatment system would helpful to decrease the metals migration during thermal treatment process of discarded LCD panels.

- **Keywords:** Thermal treatment; LCD panel; Polarizer effect; Metals migration and speciation transformation; Potential risk

Jinxuan Xu, Veeriah Jegatheesan, Ravi Raveendran, Bryan Chatelier. *Option study to remove Mn(2+) by KMnO4 at a water treatment plant*. Pages 327-337.

Thermal stratification in reservoirs resuspends manganese (Mn) from the bottom layer to the top layer. When the water from this top layer is taken for the treatment of potable water supply, removal of Mn becomes essential. The Foster Water Treatment Plant (FWTP) situated in South Gippsland, Australia applies KMnO4 to remove Mn. It also uses powdered activated carbon (PAC) remove odour causing compounds such as geosmin and 2-Methyl-Isoborneol (MIB). This study aims to investigate an optimal KMnO4 dosing strategy including (i) optimizing the dosage of KMnO4, (ii) dosing order of PAC and soda ash/KMnO4 and (iii) the retention time required for the oxidation of Mn(2+) by KMnO4 and for the adsorption by PAC. The results showed that (a) the removal rate of [Mn(2+)+Mn(7+)] in the filtered water increased with higher dosage of KMnO4 in both dosing orders; (b) the removal of Mn(2+) neither at the entry point (after adding PAC and KMnO4) nor in the filtered water was impacted significantly by the increase in the dosage of KMnO4 when the dosage was 4 times higher than the concentration of Mn(2+) present in the raw water; (c) for a given KMnO4 dosage, there were no significant changes in the removal of [Mn(2+)+Mn(7+)] and Mn(2+) at the entry point and in the filtered water when the retention times ranged from 5 to 15 min in both order of dosing; (d) for a given KMnO4 dosage, Order 1 had higher removal of total Mn compared to that of Order 2 (Order 1 is the addition of PAC before adding soda ash to increase the alkalinity and then adding KMnO4 and Order 2 is the addition of soda ash and KMnO4

before adding PAC); (e) higher removal of [Mn(2+)+Mn(7+)] was obtained in Order 2 compared to that of Order 1 for a given dosage of KMnO4; (f) for the Mn(2+), the removal did not change with the order of dosing of KMnO4 and PAC. It could be concluded that dosing KMnO4 with four times the concentration of Mn(2+) present in raw water and providing 10 min retention time for the oxidation can be a suitable dosing strategy in FWTP and dosing order has no impact on achieving the Mn removal required.

- **Keywords:** Dosage; Dosing order; Drinking water treatment; KMnO4; Mn removal; Powder activated carbon

Alessio Misuri, Valerio Cozzani. *A paradigm shift in the assessment of Natech scenarios in chemical and process facilities*. Pages 338-351.

Complex cascading events might arise from the interaction between natural hazards and technological installations handling hazardous substances, leading to the so called Natech scenarios. Recent severe Natech events evidenced that the accident progression was initiated by the lack of operability of auxiliary systems and utilities available in the plant, and that the unavailability of safety systems in place was a key factor in accident development. These features of Natech scenarios are not captured by the current risk assessment procedures, which mainly focus on the release of hazardous substances caused by the structural damage of equipment. Starting from the lessons learnt from two complex Natech events, the Arkema accident and the Fukushima nuclear disaster, a paradigm shift towards a comprehensive assessment of Natech risk is proposed with the support of an innovative holistic framework addressing the identification and characterization of both "direct" Natech scenarios due to equipment damage, and of "indirect" Natech scenarios generated by the failure of auxiliary systems and utilities. The specific role of the modification of safety system performance during Natech events in the escalation of accident consequences is also addressed. Categories of hazardous substances having critical properties which may lead to major accidents in case of utility system failure were identified, in order to support the identification of "indirect" Natech scenarios. The specific methods and tools available to accomplish each step of the proposed framework are discussed, along with the main open issues and future research needs.

- **Keywords:** Natech; Hazard identification; Quantitative assessment framework; Safety barriers; Utilities

Zeren Jiao, Chenxi Ji, Yue Sun, Yizhi Hong, Qingsheng Wang. *Deep learning based quantitative property-consequence relationship (QPCR) models for toxic dispersion prediction*. Pages 352-360.

It is crucial for emergency responders to makes a quick and accurate prediction of toxic chemical dispersions, which can lead to massive injuries and casualties. In this study, a toxic dispersion database is constructed by PHAST simulations, which consist of 30,022 toxic release scenarios of 19 chemicals. A quantitative consequence prediction model is then developed based on this database to efficiently and accurately predict dispersion downwind distances. Random forest, gradient boosting, and deep neural network algorithms are implemented and compared to find the best performing method for the model construction. The deep neural network is found to have the highest accuracy with the test set R2 higher than 0.994 and RMSE less than 0.1 for all key dispersion ranges. The developed toxic dispersion prediction models can be used to quickly generate instant toxic dispersion range estimations for any toxic chemicals at much lower computational costs.

- **Keywords:** Machine learning; Deep learning; Consequence modeling; Toxic dispersion; Deep neural network

Si Zou, Hongqiang Li, Lifang Liu, Shuang Wang, Xiaofeng Zhang, Guoqiang Zhang. *Research on improving comprehensive properties of a new sawdust composite insulation material by torrefaction*. Pages 361-374.

Preparing insulation materials from biomass waste is an economic and effective method of resource utilization. In this work, an eco-friendly sawdust composite insulation material was produced with its fire resistance improved by torrefying the biomass and adopting fireproof geopolymers as inorganic binders. Raw sawdust, as the fire-proof weakness, was torrefied to increase the ignition point before being added to the biomass composite insulation materials. With the increase of torrefaction temperature or residence time, the ignition point of the torrefied sawdust increased from 270 °C to 360 °C when the solid yield decreased from 95 % to 34 % For the sawdust composite insulation materials, the best comprehensive performance was achieved with the solid yield of torrefied sawdust being 60 %, and the corresponding values of thermal conductivity, density, and compression strength were 0.087 W/(m.K), 430.8 kg/m3 and 0.97 MPa, respectively. Furthermore, the composite insulation materials can maintain structural integrity under high-temperature flame spraying and obtain a satisfactory carbon sequestration capacity. Due to the advantages of environmental protection, high fire resistance, and low thermal conductivity, the torrefied sawdust composite insulation material has good application prospects in buildings.

- **Keywords:** Torrefied sawdust; Fire resistance; Biomass insulation materials; Forestry waste; Environmental protection

Ushtar Arshad, Syed Ali Ammar Taqvi, Azizul Buang, Ali Awad*. SVM, ANN, and PSF modelling approaches for prediction of iron dust minimum ignition temperature (MIT) based on the synergistic effect of dispersion pressure and concentration*. Pages 375-390.

Data-driven models for predicting fire and explosion-related properties have been improved greatly in recent years using machine-learning algorithms. However, choosing the best machine learning approach is still a challenging task. Therefore, in this study, the predictability comparisons have been made with the different machine learning methods used to model the MIT for iron dust. The MIT of iron dust was determined using the Godbert-Greenwald furnace for seventy unique combinations of dispersion pressures and dust concentrations. The data has been divided into 'Training Set' and 'Testing Set'. The implementation and efficacy of machine learning and statistical approaches have been demonstrated through real-time experimental results. The support vector machines (SVM) regression models were trained with various kernel functions to enhance the performance of the resultant model. The cubic kernel function was found suitable for training SVMs. Besides, a feed-forward artificial neural network with the backpropagation algorithm and a polynomial surface fit model have also been developed to predict the MIT. For statistical phenomena, such as MIT, predictive modelling based on real-time experimental data is critical. If an accurate estimate of the combustible dust's minimum ignition temperature is confirmed, it is possible to ensure that the temperatures of the surrounding hot surfaces do not rise to that level, preventing an explosion. An overall comparison of predictive models has been given with unseen test data set. All the trained models yielded comparable results with unseen test data set. However, the SVM model with Bayesian optimizer approach can effectively assess the risk of ignition based on dust MIT under the influence of dispersion pressure and dust cloud concentration among all the approaches adopted in this study.

- **Keywords:** MIT; Iron dust; Artificial neural networks; Support vector machines; MIT apparatus; Dust explosion

Camilla Di Marcantonio, Agostina Chiavola, Silvia Paderi, Valentina Gioia, Marco Mancini, Tommaso Calchetti, Alessandro Frugis, Simone Leoni, Giancarlo Cecchini, Massimo Spizzirri, Maria Rosaria Boni. *Evaluation of removal of illicit drugs, pharmaceuticals and caffeine in a wastewater reclamation plant and related health risk for non-potable applications*. Pages 391-403.

The present study aimed at determining the presence and removal rate achieved through the main treatment stages of a full-scale wastewater reclamation plant for some classes of Organic Micropollutants. Furthermore, the human health risk due to the reuse of the final effluent containing residual concentrations of these pollutants for non-potable applications was assessed. The 8-months monitoring campaign on the influent and effluent of the treatment stages of the plant highlighted that the main removal took place in the bioreactor, reaching median removal of 99 %, 97 %, 60 % 76 %, 71 %, 96 % and 100 %, for benzoylecgonine, cocaine, methamphetamine, trimetoprim, sulfadiazine, ketoprofene and caffeine, respectively. This result was also confirmed by the application of the principal component analysis. A further abatement, although slight, occurred in the tertiary compartment (made up by filtration, UV disinfection and chlorination) for sulfamethoxazole, trimethoprim and ketoprofen, determining a final median removal of 50 %, 94 % and 98 %, respectively. A significant correlation between the removal processes of the investigated organic micropollutants and the traditional water quality parameters was also found out. The human health risk for incidental ingestion and dermal contact resulted to be always below 1 under average and worst scenarios, which indicates that the risk can be considered acceptable.

- **Keywords:** Contaminants of emerging concern; Human health risk; Organic micropollutants; Reclamation; Wastewater reuse; Wastewater treatment plant

Pouran Makhdoumi, Milad Naghshbandi, Kamyar Ghaderzadeh, Mahsa Mirzabeigi, Ahmadreza Yazdanbakhsh, Hooshyar Hossini. *Micro-plastic occurrence in bottled vinegar: Qualification, quantification and human risk exposure*. Pages 404-413.

Micro-plastics (MPs) have recently been detected in the environmental medium and in a lot of products, particularly in the products consumed by humans. In the present study, the contamination of vinegar containers by MPs was investigated from nine popular brands consumed in Iran. Using a Nile Red staining and stereomicroscope analysis, MPs were detected in all sample brands. The most MPs were found in the shape of fragment (94 %), while only a few was in the fiber shape (6%). MPs were identified by using FTIR stereoscopy and PE and HDPE were founded as the most likely polymers. The annual human exposure to average concentration of MP was approximately estimated as 4.9 and 21.2 mg/kg/bw/year corresponding to optical detection for adult and children, respectively. While the annual intake was around 4.7 and 20.7 mg/kg/bw/year according to fluorescence observation. The findings of the present study showed that the MPs particles releasing can occur from food plastic container into the content like the vinegar.

- **Keywords:** Vinegar; Microplastics; Red Nile; Plastic bottles

Tássia L.S. Quaresma, Tatiele D. Ferreira, Sávio S.V. Vianna. *A hybrid BML-fractal approach for the mean reaction rate modelling of accidental gas explosions in partially confined obstructed geometries*. Pages 414-426.

We propose a new approach to model the mean reaction rate of premixed turbulent flames when simulating accidental gas explosions with computational fluid dynamics (CFD). The combination between Bray–Moss–Libby (BML) approach and the fractal

concept was evaluated. The fractal concept is used for closing the integral length scale of wrinkling in the BML formulation replacing the utilisation of empirical functions. The proposed expression accounts for the effect of local length scales of turbulence on the flame front via the fractal outer and inner cut-offs, which were taken respectively as the integral length scale of turbulence and the Gibson length scale. The initial laminar phase of flame propagation is described by a laminar combustion model and the onset of the transition from the laminar to turbulent combustion is assumed to take place at a threshold value of the turbulent Reynolds number. The approach is implemented and evaluated within an in-house developed code called STOKES (Shock Towards Kinetic Explosion Simulator) that solves the full set of Navier–Stokes equations. The equations are parameterised according to the porosity distributed resistance (PDR) method in which the porous mesh accounts for the presence of small obstacles that are responsible for turbulence generation during an explosion. Simulations are carried out for vented explosions of both methane–air and propane–air mixtures in partially obstructed chambers. Results are compared with experimental data, FLACS simulations and a typical model for the length of wrinkling which uses an empirical function instead of the fractal approach. Comparisons lead to overall good agreement, indicating that the proposed model can be used in numerical simulations of accidental explosions to support consequence modelling in the framework of risk analysis.

- **Keywords:** BML reaction rate model; Premixed turbulent combustion; Fractal approach; Initial laminar phase; Gas explosion; CFD

Xuewen Cao, Kairan Yang, Jiang Bian. *Investigation of CO2 hydrate slurry flow characteristics with particle dissociation for carbon storage and transportation*. Pages 427-440.

CO2 capture and storage technology is an effective method to mitigate the greenhouse effect and hydrate slurry is a high-efficiency way of CO2 transportation. In this study, in order to further reduce the cost and improve the transportability, a new CO2 hydrate slurry transport mode which allows a small part of hydrate particles to dissociate during flow process is proposed. To investigate the CO2 hydrate slurry flow characteristics and particle micro behaviors, a multiphase flow model coupled with hydrate dissociation kinetic model and population balance model is established. Experimental results are used to verify this integrated model. Furthermore, the effects of hydrate dissociation on CO2 transportability are also analyzed. The results indicate that the dissociation rate of hydrate during flow process can be divided into rapid dissociation stage and weakened dissociation rate stage. The agglomeration of hydrate particle can reduce the total surface area, further resisting the dissociation rate. The hydrate particle size experiences a process of growing to dynamic balance. The hydrate dissociation can decrease the mean viscosity of CO2 hydrate slurry flow, which can reduce the pressure drop and energy loss compared with the flow without hydrate dissociation. The generated bubbles can accelerate the CO2 hydrate slurry flow, increasing the transportability and reducing the risk of hydrate blockage in pipe induced by agglomeration.

- **Keywords:** CO2 capture and storage; Hydrate slurry; CO2 transportation; Particle behaviors; Flow assurance

Avni Jain, Sonu Kumari, Swati Agarwal, Suphiya Khan. *Water purification via novel nano-adsorbents and their regeneration strategies*. Pages 441-454.

Nanotechnology has immensely contributed for the treatment of contaminated water with the development of nano-adsorbents. In last few years, the demand of nano-adsorbents in the water industry has grown rapidly. Therefore, regeneration of utilized adsorbents has become a foremost issue as they are often hazardous. Different techniques for regeneration of adsorbents have been developed such as thermal, steam, chemical,

microwave-assisted, electrochemical, and bio-regeneration. For this, different parameters and factors should be taken into account for efficient adsorbents regeneration such as pH, temperature and time. These applied regeneration strategies play a major role in the improvement of adsorbent's lifetime, adsorption cycles and replacement rate. Moreover, recovery of precious metals can only be possible by desorption of the metals adsorbed through suitable regeneration techniques. Thus, regeneration can contribute towards the balance of ecology and environmental safety by enhancing the application cycles. This comprehensive review is an attempt to help the scientific community working on adsorption studies to take up research initiatives required to address the feasible recovery methods of adsorbed materials from the used adsorbents, to study the possible reuse of the desorbing agents, and to choose a suitable desorbing/regenerating agent for a particular application.

- **Keywords:** Adsorbents; Adsorption; Regeneration; Nanotechnology; Desorption

Xin Wang, Zhonghua Wang, Xinyuan Yin, Haiqian Zhao, Chuanyan Wu, Xiaoyan Liu. *Promotion of NO oxidation through H2O2 thermal decomposition using a metal surface*. Pages 455-461.

Considerably slow H2O2 evaporation leads to a decrease in the oxidation ratio of NO through H2O2 thermal decomposition. Therefore, the metal surfaces of Copper h62, Aluminium 5052, Steel 201, and Steel q235 were used to promote H2O2 thermal decomposition and NO oxidation. The effects of reaction temperature, H2O2 solution concentrations, H2O2:NO ratios, and metal surface inclination angles on NO oxidation were explored through H2O2 thermal decomposition. The evaporation and decomposition rates of H2O2 significantly influenced NO oxidation. After the addition of metal surfaces to the reactor, the NO oxidation ratio considerably enhanced, and NO concentration fluctuations disappeared under most conditions. The hydrophilicity of the metal surfaces can help the H2O2 solution spread rapidly on metal surfaces. The liquid film thickness decreased, which led to an increase in the H2O2 evaporation rate. Consequently, NO oxidation ratios improved. Metal surfaces promoted H2O2 decomposition to produce OH, and relatively more NO was oxidised. The highest NO oxidation ratio was 87 %, which was acquired using the 15 % H2O2 solution at 500 ℃. When temperature was higher than 300 ℃, NO oxidation ratios on different metal surfaces were similar. The inclination angle θ of metal surfaces can considerably affect NO oxidation ratios. When the metal surface was horizontal, the NO oxidation ratio was higher than that when metal surface was placed at other angles, and the oxidation effect of NO was relatively more stable. The longer the droplets stayed on metal surfaces, the smaller were the NO concentration fluctuations.

- **Keywords:** H2O2 decomposition; Evaporation rate; Metal surface; Inclination angle

Hongqiu Zhu, Qiling Wang, Fengxue Zhang, Chunhua Yang, Yonggang Li. *A prediction method of electrocoagulation reactor removal rate based on Long Term and Short Term Memory–Autoregressive Integrated Moving Average Model*. Pages 462-470.

In the process of electrochemical wastewater treatment, the removal rate of electrocoagulation reactor will be affected by various factors such as the pH value of wastewater solution, the current density, the wastewater flow rate and the initial concentration of heavy metal ions. Therefore, this study proposes a prediction method of the removal rate of the electrocoagulation reactor based on deep learning Long and Short-Term Memory (LSTM) network combined with the Autoregressive Integrated Moving Average Model (ARIMA) commonly used in engineering. Firstly, according to the concentration of heavy metal ions in the outlet and inlet solution of the reactor, the

calculation formula for the removal rate of the reactor is defined. Secondly, in order to deepen the LSTM network model to analyze and learn the change trend of the historical removal rate data, the gradient value of the historical removal rate of the reactor before and after the change is extracted as its change feature value, and this feature value is taken as one of the input variables of the LSTM network model. Comprehensive analysis considered important factors such as the historical removal rate value of the reactor, the initial pH value of the wastewater solution, the voltage and current value, and the wastewater flow rate as the input variables of the LSTM deep learning network. The predicted value of the removal rate of electrocoagulation reactor is concluded by testing the combination of activation function and the number of fully connected layers, and the error compensation of the predicted value is carried out by using the ARIMA model. The effectiveness of the proposed method is verified by the industrial data collected from a wastewater treatment plant.

- **Keywords:** Electrocoagulation; LSTM; Feature extraction; Error compensation

Prashanth K, Amjad Shaik, Srinivasa Rao T, Pavan Bharadwaja B. *Experimental investigation of argon gas induction on diesel engine performance and emission characteristics: A comprehensive study on de-NOx techniques*. Pages 471-481.

Diesel engines are considered as the most efficient type of internal combustion engines that are widely used for transportation and power generation around the world. However, NOx emissions have always been a major concern for the development of clean diesel vehicles. As this is the global byproduct of high temperature combustion, the dwindling of NOx from emissions is required in stationary as well as mobile applications. Induction of argon into the combustion chamber is one of the promising methods to reduce NOx emissions. This paper mainly focuses on the influence of argon atmosphere in diesel engine induction system and its effect on reduction of oxides of nitrogen and carbon dioxide emissions. Experimental investigation has been carried out on a single cylinder diesel engine with varying percentages of argon gas induction from 0 to 12 % in the intake manifold. The results revealed that the induction of argon at different dilution ratios has potential to significantly reduce the formation of carbon dioxide and oxides of nitrogen. It is also observed that, a slight reduction in exhaust gas temperature with no much variation in performance parameters. This paper has also reviewed various de-NOx techniques used for diesel vehicles in detail.

- **Keywords:** Argon gas; Diesel engine; Oxides of nitrogen; Specific heat ratio

Nallapaneni Manoj Kumar, Mazin Abed Mohammed, Karrar Hameed Abdulkareem, Robertas Damasevicius, Salama A. Mostafa, Mashael S. Maashi, Shauhrat S. Chopra. *Artificial intelligence-based solution for sorting COVID related medical waste streams and supporting data-driven decisions for smart circular economy practice*. Pages 482-494.

Waste generation is a continuous process that needs to be managed effectively to ensure environmental safety and public health. The recent circular economy (CE) practices have brought a new shape for the waste management industry, creating value from the generated waste. The shift to a CE represents one of the most significant challenges, particularly in sorting and classifying generated waste. Addressing these challenges would facilitate the recycling industry and helps in promoting remanufacturing. But in the COVID times, most of the generated waste is getting mixed with conventional waste types, especially in the global south. The pandemic has resulted in colossal infectious waste generation. Its handling became the most significant challenge raising fears and concerns over sorting and classifying. Hence, this study proposes an Artificial Intelligence (AI) based automated solution for sorting COVID related medical waste streams from

other waste types and, at the same time, ensures data-driven decisions for recycling in the context of CE. Metal, paper, glass waste categories, including the polyethylene terephthalate (PET) waste from the pandemic, are considered. The waste type classification is done based on the image-texture-dependent features, which provided an accurate sorting and classification before the recycling process starts. The features are fused using the proposed decision-level feature fusion scheme. The classification model based on the support vector machine (SVM) classifier performs best (with 96.5 % accuracy, 95.3 % sensitivity, and 95.9 % specificity) in classifying waste types in the context of circular manufacturing and exhibiting the abilities to manage the COVID related medical waste mixed.

- **Keywords:** Medical waste streams; Smart circular economy; COVID waste management; Waste sorting; Feature fusion; Machine learning

Neha Parveen, Lubna Siddiqui, Md Nawaj Sarif, Md Safikul Islam, Nazreen Khanam, Sk Mohibul. *Industries in Delhi: Air pollution versus respiratory morbidities*. Pages 495-512.

Industrialization has been contributing to the economic development of countries all over the globe but on the other side of the coin, it is also causing deterioration of the environment as well as human health. Air pollution in industrial areas has emerged as a hasten issue in recent years due to its aggravated effects on health and wellbeing. The objectives of the study are to analyze the concentrations of air pollutants (PM10, PM2.5, NO2 & CO) in industrial areas of Delhi and to assess the association among meteorological variables, air pollutants, and respiratory diseases of industrial workers and their family members. To map these pollutants concentration, Kriging and Inverse Distance Weighted (IDW) interpolation techniques were employed. The results showed that several industrial areas were cloaked with all these four pollutants in varied ranges and different seasons. The increase in the number of registered and operating industries in Delhi, and the consequential rise in the air pollutants' concentrations followed the quadratic polynomial trend. Spearman's rho correlation technique revealed that the respiratory disease entries of workers and their families depicted a statistically strong negative correlation with temperature, rainfall, and wind speeds while a strong positive association with PM2.5, NO2, and CO.

- **Keywords:** PM10; PM2.5; NO2; CO; Industrial areas; Respiratory diseases

Safoura Vaez, Keikhosro Karimi, Safoora Mirmohamadsadeghi, Azam Jeihanipour. *An optimal biorefinery development for pectin and biofuels production from orange wastes without enzyme consumption*. Pages 513-526.

Orange wastes, including peel and pulp, were used as a biorefinery feedstock to produce pectin, ethanol, and biogas. The orange wastes were subjected to dilute acid treatment with sulfuric acid (1% w/v) at 94, 100, 140, and 180 °C for 60, 30, and 0 min. The sulfuric acid treatment was performed for pectin extraction, sugars hydrolysis, and lignocellulose pretreatment. The pectin was extracted from the hydrolysate, the liquor was used to produce ethanol, and the pretreated solid was anaerobically digested to produce biogas. The highest pectin extraction yield was 24.7 % (w/w) from orange peel and 23.7 % (w/w) from pulp, which was obtained from the supernatants of treatment at 94 °C for 60 min. Fourier transfer infrared spectrometer results confirmed the similar characteristics of the extracted pectin to a commercial product. The galacturonic acid content (an indicator of pectin purity) of pectin extracted from orange peel was 70.2 % and from orange pulp was 69.9 %, at the optimum conditions. The pectin obtained from the acid treatment at 94 °C for 60 min had a degree of esterification higher than 69 %, whereas it was less than 45 % for that obtained after treatment at 140 °C for 30 min.

The maximum ethanol yields of 81.5 % (from peel) and 82.9 % (from pulp) were achieved from the hydrolysate of the acid treatment at 140 °C for 30 min. The highest methane yields were 176.8 mL/g volatile solids (from the untreated peel) and 191.8 mL/g volatile solids (from the untreated pulp). Overall, the maximum total product value was 2,472.9 USD/t orange wastes, which was achieved from dilute acid treatment at 94 °C for 60 min. At the optimal conditions for high production of pectin, without any enzyme consumption, 244 kg of pectin, 26.5 L of ethanol, and 36 m3 of methane were produced from 1 t of orange wastes.

- **Keywords:** Ethanol; Methane; Orange waste; Dilute acid pretreatment; Pectin

Huayong Zhang, Yudong Cao, Yonglan Tian, Lei Zheng, Hai Huang. *Metal speciation distribution of anaerobic fermentation with alfalfa grass harvested from abandoned iron mine and the influence of metals addition*. Pages 527-535.

Metal-contaminated plants after phytoremediation provide organic matter and trace metals for anaerobic fermentation. In this study, alfalfa straw harvested from an abandoned iron mine was used for anaerobic fermentation. The variation of metal speciation during the anaerobic fermentation process and the influences on fermentation parameters were investigated. The results showed that the group adding alfalfa increased the peak daily biogas yield by 33.40 % compared to the group with cow dung only. Fe in the fermenter was predominated by the soluble and the residual fraction. Cu was transformed from soluble Cu to residual Cu with the fermentation progressed. On the 13th day of fermentation, the percentage of soluble Fe decreased while the percentage of soluble Cu, Ni and Zn increased which induced the daily biogas yields peak. Metal speciation was correlated to the fermentation parameters. Daily biogas yields were negatively correlated to the acid-extractable fraction of Ni and Zn ($p < 0.05$). pH was negatively correlated to the soluble Cu, the acid-extractable fraction of Cu and Zn ($p < 0.05$), while positively correlated to the reducible and oxidizable Fe ($p < 0.01$). Further adding metals promoted the biogas production of alfalfa by bringing forward the daily biogas peak and increasing the peak yields. In particular, adding Cu only produced more biogas than adding other metals (single or multiple). Exogenous metals addition generally resulted in more acid-extractable fraction of Cu, Ni and Zn, i.e. the mobility of these metals increased. 19 % of Fe was activated into acid-extractable fraction after the addition of Ni. The results of this study are expected to provide references for the reutilization of contaminated biomass and optimizing the metal contained fermentation process.

- **Keywords:** Metal speciation; Anaerobic fermentation; pH values; Spearman correlation analysis

Yanni Zhang, Pan Shu, Fangyan Zhai, Shaokang Chen, Kai Wang, Jun Deng, Furu Kang, Lele Li. *Preparation and properties of hydrotalcite microcapsules for coal spontaneous combustion prevention*. Pages 536-548.

Microcapsule materials are a new type of composite fire-extinguishing material that show good effects in preventing the spontaneous combustion of coal. In this paper, polyethylene glycol 6000 (PEG6000) was selected as the wall material, and hydrotalcite (LDHs) was selected as the core material. Microencapsulated LDHs samples with different core-to-wall ratios were prepared by melting dispersion and condensation. Scanning electron microscopy coupled with energy dispersive spectroscopy (SEM-EDS), Fourier transform infrared spectroscopy (FTIR), thermogravimetry/differential scanning calorimetry (TG/DSC) and other experiments were used to characterize the surface morphology, dispersion, coating, pyrolysis and other characteristics of the microcapsules.

On this basis, the microcapsules were mechanically mixed with a coal sample to prepare a chemically inhibited coal sample. Based on TG/DSC experiments, the effect of microcapsules with different core-to-wall ratios on the characteristics of coal spontaneous combustion was studied. Combined with thermokinetic parameters, the inhibition mechanism of the microcapsules with different core-to-wall ratios on coal spontaneous combustion was analyzed. The results showed that LDH-PEG6000 microcapsules were successfully prepared. The thermal reactivities and inhibition mechanism of microcapsules with different core-to-wall ratios were different, and the best effect was obtained when the core-to-wall ratio was 1:5. This microcapsule material can reduce the weight loss rate and heat release of coal, increase the critical temperature and maximum weight loss rate temperature by 8.8 °C and 33.6 °C, respectively, and increase the apparent activation energy of water evaporation and gas desorption stage by 13.42 kJ/mol and the thermal decomposition stage and combustion stage by 88.64 kJ/mol. Resistance microcapsules can effectively inhibit the coal spontaneous combustion reaction In addition, this research provides new ideas for solving the problem of coal spontaneous combustion in the goaf caused by the fully mechanized top coal caving technology and enriches the technical means of fire prevention.

- **Keywords:** Coal spontaneous combustion; Resistance microcapsules; Different core-to-wall ratios; Characteristic temperature point; Activation ability

Rongliang Pan, Guoqing Zhu, Gang Xu, Xin Liu. *Experimental analysis on burning rate and temperature profile produced by pool fire in a curved tunnel as a function of fire location*. Pages 549-567.

To analyze the influence of a curved ceiling and fire location on the combustion characteristics in a utility tunnel, the burning rate and temperature profile produced by a pool fire beneath a curved ceiling were investigated experimentally and theoretically. The results showed that oxygen supply and heat feedback from the surrounding form a competitive mechanism, determining the evolution of the burning rate. A qualitative analysis was performed to elucidate this competitive mechanism. With the fire source moving close to the sidewall, the positive influence from the heat feedback is is gradually compensated for by the negative influence from oxygen supply limitation. Moreover, it was inferred that the magnitude of decline of the burning rate near the wall has a positive correlation with heat release rate of the fire source. A characteristic inclined angle was defined to replace the changing angle of the curved ceiling along the ceiling jet path. Based on the definition of the characteristic 'inclined angle' concept, the relationship between the temperature profile beneath the curved ceiling centerline, tunnel height and horizontal position from fire source was unified by an empirical model. The maximum temperature delay beneath the curved ceiling centerline produced by the pool fire was analyzed by radial flow and one-dimensional flow. The proposed models for radial flow and one-dimensional flow were validated and could effectively predict the maximum temperature delay, which can be applied in utility tunnel's fire protection engineering.

- **Keywords:** Curved ceilings; Pool fire; Burning rate; Temperature profile; Fire location

Ramiro Picoli Nippes, Paula Derksen Macruz, Gabriela Nascimento da Silva, Mara Heloisa Neves Olsen Scaliante. *A critical review on environmental presence of pharmaceutical drugs tested for the covid-19 treatment*. Pages 568-582.

On March 11, 2020, the World Health Organization (WHO) declared COVID-19 a pandemic. The outbreak caused a worldwide impact, becoming a health threat to the general population and its professionals. To date, there are no specific antiviral

treatments or vaccines for the COVID-19 infection, however, some drugs are being clinically tested. The use of these drugs on large scale raises great concern about their imminent environmental risk, since the elimination of these compounds by feces and urine associated with the inefficiency of sewage treatment plants in their removal can result in their persistence in the environment, putting in risk the health of humans and of other species. Thus, the goal of this work was to conduct a review of other studies that evaluated the presence of the drugs chloroquine, hydroxychloroquine, azithromycin, ivermectin, dexamethasone, remdesivir, favipiravir and some HIV antivirals in the environment. The research indicated the presence of these drugs in the environment in different regions, with concentration data that could serve as a basis for further comparative studies following the pandemic.

- **Keywords:** Pandemic; SARS-CoV-2; Medicaments; Emerging micropollutants; Environmental pollution

Maria A. Zoran, Roxana S. Savastru, Dan M. Savastru, Marina N. Tautan, Laurentiu A. Baschir, Daniel V. Tenciu. *Exploring the linkage between seasonality of environmental factors and COVID-19 waves in Madrid, Spain*. Pages 583-600.

Like several countries, Spain experienced a multi wave pattern of COVID-19 pandemic over more than one year period, between spring 2020 and spring 2021. The transmission of SARS-CoV-2 pandemics is a multi-factorial process involving among other factors outdoor environmental variables and viral inactivation.This study aims to quantify the impact of climate and air pollution factors seasonality on incidence and severity of COVID-19 disease waves in Madrid metropolitan region in Spain. We employed descriptive statistics and Spearman rank correlation tests for analysis of daily in-situ and geospatial time-series of air quality and climate data to investigate the associations with COVID-19 incidence and lethality in Madrid under different synoptic meteorological patterns. During the analyzed period (1 January 2020-28 February 2021), with one month before each of three COVID-19 waves were recorded anomalous anticyclonic circulations in the mid-troposphere, with positive anomalies of geopotential heights at 500 mb and favorable stability conditions for SARS-CoV-2 fast diffusion. In addition, the results reveal that air temperature, Planetary Boundary Layer height, ground level ozone have a significant negative relationship with daily new COVID-19 confirmed cases and deaths. The findings of this study provide useful information to the public health authorities and policymakers for optimizing interventions during pandemics.

- **Keywords:** COVID-19 disease; Synoptic atmospheric circulation; Air quality; Seasonal variability of climate and Planetary Boundary Layer height; NOAA satellite data

João Lincho, João Gomes, Marek Kobylanski, Beata Bajorowicz, Adriana Zaleska-Medynska, Rui C. Martins. *TiO2 nanotube catalysts for parabens mixture degradation by photocatalysis and ozone-based technologies*. Pages 601-613.

The evolution of the analytical techniques allowed the detection of pollutants so called contaminants of emerging concern (CEC). Water scarcity is a reality lived by some populations. Thus, water reuse is mandatory to minimize this problematic. This implies that wastewater treatments must be improved. The Advanced Oxidation Processes (AOP) such as photocatalysis and ozonation can be suitable solutions for CECs abatement. Also, TiO2 powder catalyst is an important material in this field. However, its powder form presents a huge obstacle for industrial application, and the solution may be to support this material. This work studies the degradation of a mixture of 3 parabens by photocatalysis, catalytic and photocatalytic ozonation using TiO2 nanotube arrays (NTs).

The studied catalysts were produced using electrolyte solutions with different ages, so the nanotubes growth ocurred at 5 (NTs_5) and 20 (NTs_20) anodization cycles. The toxicological assessment for the initial mixture, final samples and along the reaction time was performed using the cress seeds Lepidium sativum and the bacteria Aliivibrio fischeri. The photocatalysis with UVA radiation led to 50 % and 35 % parabens removal for NTs_5 and NTs_20 catalysts. This can be related to the different dimensional characteristics of the nanotubes. Ozone technologies led to total parabens degradation with an improvement when catalytic ozonation was applied. The use of NTs as catalysts in ozonation also reduced the transferred ozone dose (TOD) required for total parabens abatement when compared to single ozonation. The main parabens degradation mechanism seems to be via direct pathway by molecular ozone. Regarding the toxicity assessment, the toxicity did not change significatively, which can be explained by the intermediate's formation.

- **Keywords:** AOP; TiO2 nanotubes; Parabens; Supported catalysts; Wastewater treatment

Ankit Dasgotra, Goutham Rangarajan, S.M. *Tauseef. CFD-based study and analysis on the effectiveness of water mist in interacting pool fire suppression*. Pages 614-629.

Accidental fires result in extensive loss of property, damage to the environment and a large number of fatalities every year. When fuel collects in the form of a pool and burns, it is termed a pool fire. Pool fires may burn in isolation – Non-interacting or as Single Pool Fires (SPFs) – or flames from multiple pool fires may interact with each other and burn in what is termed as Multiple Pool Fires (MPFs). Even as single pool fires (SPFs) are difficult to control, interacting flames due to multiple pool fires (MPFs) are even more difficult to extinguish. Compared to SPF, MPFs tend to have much higher flames and are reported to have extraordinary thermal intensity. Accidental pool fires in warehouses, commercial and residential buildings may interact, giving rise to interacting pool fires (MPFs). The commonly used technique to suppress fires in enclosures such as warehouse, commercial or residential buildings is to use sprinklers. Hence, this study reports the numerical simulations performed to analyse the effectiveness of water-mist sprinklers in extinguishing MPFs. The related CFD coding and simulations were performed using Fire Dynamics Simulator (FDS), FDS tools like Pyrosim (pre-processor) and Smokeview (post-processor) packages. The effect of the ratio of the separation distance between the pools (S) to the diameter (D) on the overall fire suppression efficiency of the water-mist sprinkler as a function of the water mist flow rate, the height of the ceiling, and sprinkler particle size are vigorously analysed in this work. The analysis presented in this article will mainly help to resolve problems associated with the effectiveness of mist-sprinkler in warehouse fires regarding process safety viewpoint.

- **Keywords:** Multiple pool fires; Fire suppression; Water mist; FDS; Sprinklers; Pressure drop

Carmen Padilla-Rascón, Juan Miguel Romero-García, Encarnación Ruiz, Inmaculada Romero, Eulogio Castro. *Microwave-assisted production of furfural from the hemicellulosic fraction of olive stones*. Pages 630-640.

Olive stone (OS) is a lignocellulosic material obtained as a coproduct in the olive oil production industry, mainly composed of hemicelluloses, with xylose accounting for 24.4 % by weight as the main sugar. In this study, an optimized process for obtaining furfural from OS was assessed. The process consists of two steps; the first one, aimed at maximizing the solubilization of xylose, was performed in an autoclave at 130 °C and 2.6 %w/v H2SO4, resulting in 83 % xylose recovery in the liquid fraction. The second step, using the optimized liquid produced previously, was carried out in a microwave reactor at 200 °C with the addition of 0.1 M FeCl3 from which a solution with 18 g/L furfural and

63.3 % yield was obtained, equivalent to almost 90 kg of furfural per tonne of processed OS. Taking into account these results along with additional advantages in comparison with other lignocellulosic materials (such as no need of a grinding stage and being already available in the olive mills), OS can be considered as a promising raw material for furfural production.

- **Keywords:** Olive biomass; Xylose; Furfural; Microwave; Optimization

Shashi Arya, Rahul Rautela, Digambar Chavan, Sunil Kumar. *Evaluation of soil contamination due to crude E-waste recycling activities in the capital city of India*. Pages 641-653.

Unempirical E-waste urban mining is beleaguered as a potential threat to the environment and human health. India is intensely imperiled as a chaotic region for approximately 95 % of immature E-waste recycling among which Delhi is the foremost hub. A field study at active E-waste recycling sites in Delhi was carried out to estimate the soil contamination due to the release of toxic elements in the vicinity areas. The geoaccumulation index, contamination factor, and ecological risk indicated that the soil was contaminated with the metals like Pb (1569.9), Cd (2.41), Zn (675.89), Ni (61.02), Cu (3846.8), & Al (9864.2) mg/kg, and Pb (2627.94), Al (8123.6 Cu (4108.7), Zn (354.18), & Cd (3.56) mg/kg which exceeded the threshold limit of WHO, respectively at both the acid leaching and open burning areas of E-waste recycling sites. For effective E-waste management at the informal E-waste recycling sites requires a cost-effective and environment-friendly treatment method. The results of the present study show the higher soil contamination due to the presence of heavy metals. Hence, there is a dire need for taking immediate actions and control measures by the policymakers and decision-makers and adopt scientific methods toward restricting the migration of metals into the surroundings. Phytoremediation and bioremediation are highly recommended to curb the accumulation of hazardous materials at the contaminated sites.

- **Keywords:** Crude recycling; E-waste effluent; Soil pollution; Heavy metals; Index of geoaccumulation; Contamination factor

Guanlong Yu, Guoliang Wang, Shitao Wang, Chunping Yang, Hong Chen, Yancong Zhu, Li'e Yu, Jianbing Li, Hossein Kazemian. *Performance promotion and its mechanism for n-hexane removal in a lab-scale biotrickling filter with reticular polyurethane sponge under intermittent spraying mode*. Pages 654-662.

Mass transfer limitations commonly challenge biofiltration for n-hexane emissions due to its high hydrophobicity. In this study, a bench-scale biotrickling filter (BTF) packed with reticulated polyurethane sponge was evaluated for n-hexane removal at various organic loading rates (OLRs) (ranging from 15 to 60 g m−3 h-1) and gas empty bed contact times (EBCTs) (ranging from 30 to 7.5 s). The obtained results show that the designed BTF can effectively remove n-hexane under intermittent spraying mode of the nutrient solution and the reticulated configuration of the packing media, which resulted in the spatial development of mycelium and enhanced mass transfer of n-hexane. The mean maximum removal efficiencies (REs) of n-hexane were 92.6 ± 0.9 %, 86.7 ± 4.8 %, and 63.8 ± 3.3 % under the OLRs of 15.67, 30.20, and 61.59 g m−3 h-1, respectively. When the BTF was operated under gas EBCTs of 30, 15, and 7.5 s, average REs of 85.9 ± 5.7 %, 44.8 ± 6.3 %, and 31.2 ± 2.5 % were achieved. The BTF also showed a superior fluctuation resistance capability and prevented excessive biofilm accumulation due to the reticular configuration of the polyurethane sponge. Results present in this study could provide an alternative consideration for the practical industrial application in treating hydrophobic VOC like n-hexane.

- **Keywords:** Biotrickling filter; n-Hexane; Filamentous bacteria; Reticular polyurethane sponge; Enhanced mass transfer

Vasudha Hasija, Pankaj Raizada, Pardeep Singh, Narinder Verma, Aftab Aslam Parwaz Khan, Arachana Singh, Rangabhashiyam Selvasembian, Soo Young Kim, Chaudhery Mustansar Hussain, Van-Huy Nguyen, Quyet Van Le. *Progress on the photocatalytic reduction of hexavalent Cr (VI) using engineered graphitic carbon nitride*. Pages 663-678.

The existence of chromium in hexavalent oxidation state is highly toxic to aquatic environment. Photocatalytic reduction of hexavalent Cr (VI) into Cr (III) has emerged as a desirable technology due to their prospect in solar energy utilization, high efficiency and low cost. Graphitic carbon nitride (g-C3N4)-based photocatalysts are ideal for Cr (VI) reduction due to their inherent features including; visible-light responsive narrow bandgap, suitable conduction band potential, high physicochemical stability, unique optical and electronic properties. Herein, various surface-interface strategies to modify g-C3N4 including heterojunction formation, doping, structural regulation, co-catalyst loading and construction of nitrogen vacancies are elaborated for improving the Cr(VI) photoreduction efficiency. The review also highlights the effect of operational reaction conditions such solution pH, g-C3N4 dosage, Cr (VI) concentration, temperature, light source, organic acid additives and co-existing ions influencing Cr (VI) reduction efficiency. Finally, we attempt to propose the existing issues based on the current research and future aspects of engineered g-C3N4 for Cr (VI) photoreduction.

- **Keywords:** Graphitic carbon nitride; Photocatalytic activity; Enhancement strategies; Cr (VI) reduction; Reaction parameters

Ke Gao, Zeyi Liu, Chengqing Wu, Jun Li, Kewei Liu, Yujiao Liu, Shengnan Li. *Effect of low gas concentration in underground return tunnels on characteristics of gas explosions*. Pages 679-691.

This study numerically investigated the effect of a very low gas concentration on a gas explosion's performance numerically using OpenFOAM. The use of the Harten–Lax–van Leer–Contact (HLLC) approximation algorithm based on the density-based solver was proposed to capture the shock wave. The process variable in XiFOAM of the OpenFOAM toolbox was used for the deflagration reaction. A gas explosion test was performed, and the numerical model with OpenFOAM was validated using the testing data. Based on the numerical investigation, the influence of a very low methane concentration on the flame and shock wave propagation law of a gas explosion was analyzed. It showed that the flame initially accelerated, followed by deceleration, and then accelerated again before slowing down. An increase in the methane concentration had an enhanced effect on the maximum overpressure ratio, which increased linearly with an increase in the methane concentration from 0 vol. % to 3.0 vol. % in the return tunnels. Increasing the explosive methane volume and concentration caused a significant increase in the flame spread distance. It was also noted that increasing the methane concentration caused a linear increase in the maximum overpressure ratio, and the methane volume and concentration both had a sensitive effects on the maximum overpressure ratio and average overpressure rising rate. The results clarified how the gas explosion law was affected by a very low gas concentration and provided theoretical support for controlling gas explosion disasters.

- **Keywords:** Coal mine; Very low gas concentration; OpenFOAM; Flame propagation; Overpressure characteristic

Hakan Çelikten, S. Levent Kuzu, Arslan Saral, Murat Aksel. *Performance evaluation of a full-scale open bed biofilter through on-site measurements and CFD analyses*. Pages 692-700.

Composting process is applied to stabilize organic solid waste. But this method releases odorous organic compounds as by-product. Several methods are employed to cope with this nuisance problem. In this study, a full-scale biofilter unit was evaluated which is used in the treatment of composting waste gas. The performance of the open bed biofilter was evaluated by measurements volatile organic compounds (VOCs) and total organic carbon (TOC) from the inlet sampling ports and the outlet of the biofilter. Different sampling points were selected at the outlet of the biofilter in order to better represent removal efficiencies (RE) and determine the variability over the biofilter surface. The average TOC removal rate was 67 ± 11 %. Fifty-six different VOCs were sampled and then quantified by GC–MS. The average inlet concentrations for the target VOCs fed to the biofilter unit in November, January, April, May, and June were 57.9, 11.51, 4.54, 5.09, and 10.26 mg m−3, respectively and the removal efficiencies for these inlet concentrations were 45 %, 62 %, 32 %, 32 %, and 40 %, respectively. The deterioration of the packing material, caused reduced removal efficiencies by the time. The VOC removal rates were lower than TOC removal rates due to the selected VOC species. Further analyses were conducted with computational fluid dynamics (CFD). The effectiveness of the waste gas distribution was evaluated. Flow distribution within the biofilter was not uniform. This was also supported by the measurement results. Regions of the biofilter volume that are close to the inlet pipe had smaller retention times, which resulted in reduced treatment efficiencies.

- **Keywords:** VOC removal; TOC; Open bed biofilter; CFD; Composting

Kayleigh Rayner Brown, Peter VanBerkel, Faisal I. Khan, Paul R. Amyotte. *Application of bow tie analysis and inherently safer design to the novel coronavirus hazard*. Pages 701-718.

This work involves the application of process safety concepts to other fields, specifically bow tie analysis and inherently safer design (ISD) to COVID-19. An analysis framework was designed for stakeholders to develop COVID-19 risk management plans for specific scenarios and receptor groups. This tool is based on the incorporation of the hierarchy of controls (HOC) within bow tie analysis to identify priority barriers. The analysis framework incorporates inherently safer design (ISD) principles allowing stakeholders to assess the adequacy of controls along with the consideration of degradation factors and controls. A checklist has also been developed to help stakeholders identify opportunities to apply the ISD principles of minimization, substitution, moderation, and simplification. This work also considers barrier effectiveness with respect to human and organization factors (HOF) in degradation factors and controls. This paper includes a collection of bow tie elements to develop bow tie diagrams for specific receptor groups and scenarios in Nova Scotia, Canada. The pandemic stage (At-Peak or Post-Peak) and its influence on different scenarios or settings is also considered in this work. Bow tie diagrams were developed for numerous receptor groups; bow tie diagrams modelling a generally healthy individual, a paramedic and a hair salon patron contracting COVID-19 are presented in this work.

- **Keywords:** Bow tie analysis; Hierarchy of controls; Inherently safer design; Human and organization factors; COVID-19

Elena Nikulina, Anna Makarova, Valery Meshalkin, Vitaly Chelnokov, Aleksey Matasov, Tatiana Avdeenkova. *Integrated chemo-phyto-ecological process for the treatment of polymetal contamination in landfill sites and the consequent soil recovery*. Pages 719-729.

Non-hazardous chemical waste and municipal solid waste (MSW) are typically disposed in landfill sites. Therefore, the soils in these sites are heavily contaminated by hazardous polymetallic substances, accompanied by biocenosis disruption. Analyses of a landfill soil in Moscow showed that the concentration of metals (As, Cr3+, Zn, Cu, Ni, and Co) exceeded the established standards, and bacteria were the dominant microorganisms in the soil. A combination of sodium salts of gibberellic acid and ammonium salt of orthochlorophenyl acetic acid showed a positive effect on soil phytoremediation. These findings lay a foundation for the application of chelate-assisted and chemo-microbe-assisted phytoextraction processes in MSW soil remediation.

- **Keywords:** Microbe-assisted phyto-extraction; Phosphorus-Containing complex; Chelate-Assisted phyto-extraction