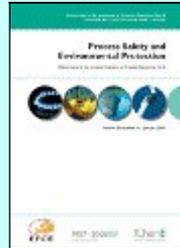


# Process Safety and Environmental Protection

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**Lang Xianming, Li Ping, Zhang Baocun, Cao Jiangtao, Guo Ying, Kan Zhe, Lu Siyu. *Localization of multiple leaks in a fluid pipeline based on ultrasound velocity and improved GWO. Pages 1-7.***

It is difficult to effectively locate the position of multiple leaks in fluid pipelines; therefore, a localization method for multiple leak positions is proposed based on ultrasound velocity and improved grey wolf optimization algorithm (GWO). First, the mathematical relationship between ultrasound velocity and the pressure signal inside a pipeline is established. Second, the ultrasound velocity is decomposed by local mean decomposition (LMD), and the inflection point of the ultrasound velocity by using a wavelet transform after denoising is extracted. Then, the simulated annealing GWO (SAGWO) method is proposed to improve the performance of GWO which is easy to converge to local optimum. Finally, the inflection time of the ultrasound velocity is obtained at the ends of a pipeline with multiple leaks, and an objective function is established to estimate the localization of the multiple leaks by SAGWO. The field experiment demonstrates that the proposed method can effectively and accurately locate multiple leak positions in a fluid pipeline.

- **Keywords:** Ultrasound velocity; Local mean decomposition; Wavelet transform; Multiple leaks localization; Simulated annealing; Grey wolf optimization algorithm

**Xinhong Li, Ziyue Han, Shangyu Yang, Guoming Chen. *Underwater gas release modeling and verification analysis. Pages 8-14.***

Accidental subsea gas releases may cause an underwater gas plume migrating from the seafloor to the sea surface, which may pose offshore fire hazards or instability of ships. Numerical simulation is an efficient approach to model the underwater gas behavior and support risk assessment. To verify the availability of numerical modeling methods for the underwater gas release, this paper establishes a small-scale experiment system to simulate the underwater gas release, and several experiments with the typical conditions are conducted to obtain the plume parameters, e.g. shape, radius and fountain height. Two CFD models, i.e. Eulerian-Eulerian and Eulerian-Lagrangian approaches, are used to reproduce underwater gas plumes in the experimental conditions. The comparison between simulations and experiments is conducted to analyze the effectiveness and the rationality of numerical modeling methods. The results indicate that simulations with two methods are overall consistent with experiments. However, a detailed comparison reflects that Eulerian-Eulerian model cannot satisfactorily capture the transition of jet to plume and the entrainment during gas rising. In contrast, the results from Eulerian-

Lagrangian model are better in agreement with experiments. This study verifies these two numerical modeling methods through a small-scale experiment. The validation against full scale tests is suggested in future work to use it as a reliable tool for risk assessment of subsea gas release incidents.

- **Keywords:** Underwater gas release; Plume; Experiment; Numerical simulation; Validation

**Geraint Thomas, Gwyn Oakley, Richard Bambrey. *Fundamental studies of explosion arrester mitigation mechanisms.* Pages 15-33.**

We report the results of laboratory investigations of the behaviour during explosion mitigation by channels typical of those used in commercial explosion arrester devices. Experimental results are presented first of shock and detonation wave interaction with a miniaturized matrix of narrow channels aligned parallel to the incoming flows. The results with a larger scale device using the same channel dimensions tested at more extreme conditions representative of overdriven detonation certification test conditions are consistent with the reduced scale laboratory measurements. To evaluate the applicability of laboratory scale evaluation of arrester elements for other types of explosion arrester, a further preliminary study is also reported with deflagration arrester elements. Finally, the present observations are interpreted in the light of published theories potentially relevant to explaining successful explosion mitigation, or otherwise, by commercial arrester devices. Using this approach, laboratory scale measurements are shown to be as a useful tool for investigating the dominant explosion mitigation mechanisms relevant to practical end user application safety devices and provide an opportunity for assisting with the design and evaluation of practical explosion, especially designs that could be supported by more comprehensive detailed CFD simulations where the supporting laboratory test configurations could also facilitate the use of more sophisticated diagnostic methods

- **Keywords:** Shock; Detonation; Deflagration; Propagation; Quenching; Narrow channels; Explosion arresters

**Shannan Xu, Bin Cao, Benjamin Bernard Uzoejinwa, Emmanuel Alepu Odey, Shuang Wang, Hao Shang, Chunhou Li, Yamin Hu, Qian Wang, Joel N. Nwakaire. *Synergistic effects of catalytic co-pyrolysis of macroalgae with waste plastics.* Pages 34-48.**

This study unveiled the synergistic effects of catalytic co-pyrolysis of the macroalgae (*Enteromorpha prolifera*) and waste plastics (HDPE) for enhanced biofuels production. Results revealed that catalytic co-pyrolysis of macroalgae (seaweeds) and waste plastics lowered greatly the high contents of the acids, oxygenates and nitrogen-containing compounds in the seaweed bio-oils, while the aromatics and light hydrocarbons contents of the bio-oils were significantly increased, owing to blending of seaweeds with co-feeding element of high hydrogen content. Results also unveiled that the existence of the co-pyrolysis synergy inhibited catalytic coking and reduced solid residues' formation. Also, the addition of HZSM-5 catalyst further improved the reaction activity, yields and selectivity of aliphatic hydrocarbons than aromatics, and reduced the activation energy without changing the reaction mechanisms. This significant reduction in activation energy can be easily observed in the results of non-isothermal kinetic analyses performed using the TGA data via five different methods: Friedman, FWO, Vyazovkin, KAS and DAEM methods, as a single kinetics-evaluation model lacks the flexibility to account for different types of materials without further modifications to reaction scheme. The FTIR-spectra of the catalytic co-pyrolysis oils were consistent with the results of the GC/MS analysis of the oils from catalytic-co-pyrolysis.

- **Keywords:** Catalytic co-pyrolysis; Macroalgae; Waste plastics; Synergistic effect; Enhanced biofuels yields

**Guang Wang, Jingsong Wang, Qingguo Xue. *Efficient utilization of waste plastics as raw material for metallic iron and syngas production by combining heat treatment pulverization and direct reduction.* Pages 49-57.**

For the clean and efficient utilization of waste plastics, an integrated flowsheet, including low temperature heat treatment pulverization and composite pellet reduction, has been proposed and the fundamental research has been conducted. The PE film could be easily pulverized by heat treatment at 250°C for 20min after mixed with coal powder (mass ratio of PE 20 % of coal). The pulverized heated mixture had better reactivity than original coal and could be used as the reducing agent of composite pellet. The reducibility of heated mixture pellet was better than coal pellet with the C/O of 1.0. The appropriate reduction temperature should be around 1100°C and the metallization degree was bigger than 90 % when reduced for 30min. The off gas of heated mixture pellet contained more H<sub>2</sub> and CO. The concentration value of H<sub>2</sub> peak of heated mixture pellet was 5 times of that of coal pellet. However, the concentration value of largest CO peak of heated mixture pellet was about 48.7 % higher than that of coal pellet. The experimental results show the possibility that the novel technology can efficiently utilize iron ore and waste plastics to produce metallic iron and syngas.

- **Keywords:** Waste plastics; Coal; Co-heat treatment; Composite pellet; Reduction

**Ronbanchob Apiratikul. *Application of analytical solution of advection-dispersion-reaction model to predict the breakthrough curve and mass transfer zone for the biosorption of heavy metal ion in a fixed bed column.* Pages 58-65.**

This work aims to apply an analytical solution of the contaminant transport model to predict the sorption's breakthrough curve and mass transfer zone of single component heavy metal ions using green macroalga, *Caulerpa lentillifera*, in a small scale cylindrical fixed-bed columns. The model was represented in a form of differential equation with two model constants which were diffusion coefficient ( $D_{eff}$ ) and linear sorption coefficient ( $k_p$ ). The linear isotherm could be well described for the sorption at a lower range of sorbate concentration while the Langmuir isotherm was suitable for a wider range of concentration. The reference set of experiments (with a bed depth of 4cm and a flow rate of 6mL/min) were used for calibrating the model to obtain the model constants. The model could be well applied to predict the breakthrough curve of varying bed depth from the reference set of experiments for the sorption of Pb<sup>2+</sup> and Cd<sup>2+</sup>. However, the model predicts slower breakthrough time than that in the experimental results when the flow rate is changed from the reference set of experiments. Three-dimensional plots and contour plots were generated to analyze the sorption behavior of metal ion in the column. The relationship between bed depth and service time (BDST) obtained from the model in this work is not linear, as often seen in the general BDST model. Both advection and dispersion processes govern the sorbate transport in the column. The mass transfer zone (MTZ) is continuously expanding along with the column length in this study. The relationship between MTZs and bed depth is also not linear.

- **Keywords:** Biosorption; Heavy metal ion; Fixed bed column; Mathematical modelling; Breakthrough curve; Mass transfer zone

**Stuart Morgan, Mark Stewart, Tasha Bennett. *Simplifying COSHH and improving chemical safety.* Pages 66-72.**

At Heineken UK, we have applied 5S principles to the legislation and guidance set out by the Health and Safety Executive (HSE) to develop a set of procedures and training materials to simplify the entire COSHH process and ensure compliance with HSE

regulations. Most notably, we have complete visibility of all COSHH assessments and safety data sheets through "COSHH Boards" and "COSHH Tubes" on each of our production lines for ease of access to critical information in an emergency. We have found these procedures and the application of 5S to drastically save time, improve COSHH assessment quality and chemical control across an entire site. The engagement and awareness of our colleagues on chemical safety has dramatically increased on our journey to a zero accident workplace.

- **Keywords:** COSHH; 5S; Chemical safety; COSHH Board; COSHH Tubes; Risk assessments

**Kai-Yu Lin, Tse-Lun Chen, Yi-Hung Chen, Pen-Chi Chiang. *Performance evaluation and environmental benefit assessment of fine particle removal using a co-current flow rotating packed bed. Pages 73-81.***

The air pollutant emission related to the anthropogenic activities affecting the environment and human health was a critical problem. Fine or ultrafine particulate matters were the major air pollutant from the industries. Thus, the high-gravity technology has holistically been applied to the integrated air pollution control due to its advances of low land demand, high mass transfer rate, low economic cost and easy operation and maintenance. In this study, the fine particle removal using a co-current flow rotating packed bed (CF-RPB) was evaluated along with different key parameters, including high gravity factor and liquid-to-gas (L/G) ratio. The obtained results suggested that CF-RPB could improve the particle removal efficiency up to 99.75 % which was increased as the high gravity factor and L/G ratio increased. In this study, a theoretical model was developed to describe that the particle size of 0.1  $\mu\text{m}$  accounted for the major concentration. Furthermore, the environmental benefit of different particle control technologies was evaluated using environmental cost accounting. The results indicated that the application of CF-RPB for particle emissions control performed greater economic feasibility than Venturi scrubber and baghouse filter. CF-RPB could also be applied to the particulate and gaseous air pollutants removal, which has more advances than the electrostatic precipitator.

- **Keywords:** Co-current flow rotating packed bed; Theoretical model; Fine particle removal; Environmental benefit assessment

**Mohit Somani, Manoj Datta, G.V. Ramana, Trichur Ramaswamy Sreekrishnan. *Contaminants in soil-like material recovered by landfill mining from five old dumps in India. Pages 82-92.***

Soil-like material (SLM) was mined from five municipal solid waste (MSW) dumps to assess its potential for reuse in earthwork projects. The contamination levels of SLM (<4.75 mm) were determined based on organic content, total soluble solids, the release of colored leachate, and heavy metals. Organic content in SLM was found to be 4–24.5 % whereas in the local soils (nearby areas) it was found to be 1–1.2 %. Total soluble solids were found to be in the range of 4820–25220 mg/kg, several times higher than that of the local soils (500–1000 mg/kg). The intensity of yellow-brown color in the water extract from SLM was observed to be 205–925 PCU while in the water extract of local soils it was found to be 25–40 PCU, highlighting the potential for release of colored leachate from SLM. Heavy metals in the SLM including chromium, copper, nickel, zinc, cadmium, and lead were found to be moderately to strongly elevated. Though SLM appears to be an attractive option for reuse, the high levels of contaminants indicate SLM would require treatment before offsite reuse.

- **Keywords:** Contaminants; Dumps; Landfill mining; Municipal solid waste; Soil-like material

**Pingyang Lyu, Ning Chen, Shanjun Mao, Mei Li. *LSTM based encoder-decoder for short-term predictions of gas concentration using multi-sensor fusion*. Pages 93-105.**

Gas is one of the most dangerous byproducts of coal in mines. Before gas accidents occur, an abnormally increased gas concentration can be observed. Therefore, a prediction of the gas concentration in coal mines is of great significance to prevent the gas accident and ensure the production safety in the mines. By calculating the Pearson correlation coefficient for the gas concentration of different sensors, the spatial correlation of the gas concentration that is monitored for each mining face is verified. We present multi-step prediction results for gas concentration time series based on the ARMA model, the CHAOS model and the Encoder-Decoder model (single-sensor and multi-sensor) and compare these results. The Encoder-Decoder model provides high robustness in a multi-step prediction and can predict the gas concentration for five different time steps. Its prediction error is significantly lower than those of the ARMA and the CHAOS models. The prediction accuracy is further improved through a fusion with information of other sensors. In this way, this study provides a novel concept and method for gas accident prevention.

- **Keywords:** LSTM; Encoder-Decoder; Gas concentration; Multi-Sensor information; Multi-Step prediction

**Yupeng Li, Weihua Cao, Wenkai Hu, Min Wu. *Diagnosis of downhole incidents for geological drilling processes using multi-time scale feature extraction and probabilistic neural networks*. Pages 106-115.**

In deep geological drilling processes, the geological environment becomes more complex with the increasing of the drilling depth; consequently, the risks of downhole incidents get higher. If not discovered in time, these downhole incidents may develop to serious drilling accidents, causing significant financial and environmental losses. In this paper, a new method is proposed to diagnose downhole incidents by extracting trend features in multi-time scales and establishing a probabilistic neural network based diagnosis model. There are two major contributions: First, a feature extraction method is proposed to produce trend features from original process signals in different time scales; Second, an incident diagnosis method based on a broad probabilistic neural network is proposed to achieve better diagnosis performance in an expanded input space. Industrial case studies are presented to demonstrate the effectiveness and practicability of the proposed method. Results show that the proposed method has superior performance in diagnosing downhole incidents for geological drilling processes.

- **Keywords:** Fault diagnosis; System safety; Geological drilling; Downhole incident; Probabilistic neural network

**Yihuan Wang, Xiangqin Hou, Peng Zhang, Guojin Qin. *Reliability assessment of multi-state reconfiguration pipeline system with failure interaction based on Cloud inference*. Pages 116-127.**

Traditional reliability theory cannot objectively describe the multi-state of the pipeline system with reliability analysis. In addition, studies on reliability modeling of the multi-state pipeline system assume that the states of each pipeline unit are independent. In this work, an efficient method was proposed to identify the performance relationship. Specifically, a model of a multi-state reconstruction system containing the decaying process and the repairing process was established. Also, a multi-state reliability modeling method was developed based on the performance degradation process of the pipeline system considering the failure interaction. Further, the Markov model of the degradation process was built to determine the relationship between the occurrence probability of

each state and the decay path. The cloud generalization function was established using cloud inference combined with the general generation function. The pipeline system can be dynamically divided by the analytic hierarchy process according to different factors affecting the degradation of pipeline performance. A numerical example was used to demonstrate the efficiency and applicability of the proposed method by comparing it with existing methods. The proposed approaches are found to be sufficient to improve risk decision and reliability analysis of the pipeline system, which better supports the reliability-informed integrity management for the whole system.

- **Keywords:** Cloud interference; Multi-state pipeline system; Failure interaction; Reconfiguration; System reliability

**G. Yu. Bivol, S.V. Golovastov. *The effect of porous coating on the flame acceleration in hydrogen–air mixture. Pages 128-139.***

Flame acceleration in the hydrogen–air mixture in the presence of porous materials was investigated experimentally. Polyurethane foam with different pore size placed on top and bottom sides of the channel was found to greatly affect flame acceleration in the channel. High-speed schlieren images showed, that polyurethane foam with larger pores leads to flame wrinkling. Dependencies of the flame velocity on the pore size were presented. It was found that final flame velocity by the end of the porous section can be up to 5 times higher while using polyurethane foam with 10 pores per inch compared to polyurethane foam with 80 pores per inch. The flame velocity in the smooth channel was lower than the flame velocity in the porous channel for all tested cases. Polyurethane foam with smaller pore size led to pressure decrease compared to solid channel. Supersonic combustion with velocity around 1600m/s was registered in the channel with PF10 on the walls. It was discovered, that the use of such a porous coating can lead to preventing the increase in the shock wave pressure during the combustion of hydrogen–air mixtures.

- **Keywords:** Hydrogen; Porous material; Flame acceleration; Polyurethane foam

**Appala Naidu Uttaravalli, Srikanta Dinda, Bhanu Radhika Gidla. *Scientific and engineering aspects of potential applications of post-consumer (waste) expanded polystyrene : A review. Pages 140-148.***

Over the past two decades, the production of expanded polystyrene (in India it is known as thermocol) has increased drastically due to its versatile applications. Consequently, the accumulation of post-consumer expanded polystyrene (EPS) in the environment has also increased alarmingly. Proper disposal and reuse of waste thermocol has become a serious global concern. In this work, a critical review has been made on various options available for the applications of waste thermocol with a focus on their process chemistry, process parameters, product yields etc. The present manuscript deals with the potential uses of waste thermocol for various applications such as to obtain value added chemicals, to use as an aggregate material in construction field, to prepare composite and porous carbon materials, and an adhesive material. From the in-depth literature analysis, it is observed that the conversion of expanded polystyrene (EPS), and the yield of liquid products mainly depends on degradation temperature, degradation duration, type of catalyst, and catalyst loading. More than 90 % EPS conversion to obtain liquid products could be achieved at a temperature range of 400–500 °C. Waste thermocol can be used in construction field to improve setting times, slump value, and water absorption capacity of concrete mixtures. In many studies, a detrimental effect of EPS on compressive strength of concrete mass has been reported. A waste thermocol can also be used to prepare porous carbon with high BET surface area (900-2700 m<sup>2</sup>/g), and high pore volume (1.2-4.2 cm<sup>3</sup>/g). Further, preparation of cost-effective adhesive from thermocol material has also been addressed in the manuscript.

- **Keywords:** Thermocol waste; Pyrolysis; Concrete mixture; Composites; Adhesive

**Shubham Chandak, Pushpito K. Ghosh, Parag R. Gogate. *Treatment of real pharmaceutical wastewater using different processes based on ultrasound in combination with oxidants. Pages 149-157.***

The discharge of effluent from the pharmaceutical industries is a major source of environmental pollution due to the toxic and at times carcinogenic nature of contaminants. The current work investigates the treatment of pharmaceutical industry effluent (PIE) using ultrasonic horn, operated individually and in combination with oxidants. Under controlled operating conditions, the effect of addition of hydrogen peroxide (ratio of COD of PIE: H<sub>2</sub>O<sub>2</sub> varied over the range from 1:1 to 1:10), ozone (flow rate of 400mg/h) and Fenton's reagent (FeSO<sub>4</sub>:H<sub>2</sub>O<sub>2</sub> ratio of 3:5) was investigated as a possible process intensification strategy. The combined approach of ultrasound, ozone and CuO catalyst (0.3g/L) as well as US + H<sub>2</sub>O<sub>2</sub> + Ozone was also studied. The combined operation of US with H<sub>2</sub>O<sub>2</sub> and Ozone resulted in a 73 % COD reduction, whereas the combination of the US, ozone and CuO catalyst gave maximum COD reduction of 92 %. The study also focused on identification of intermediate products formed during the PIE treatment. The component analysis of PIE before and after treatment was carried out by high-resolution liquid chromatography-mass spectroscopy (HR-LCMS). The research work has clearly established that cavitation in combination with other AOPs can be effectively used for the treatment of PIE with a significant increase in the extent of COD reduction for the combination approach.

- **Keywords:** Pharmaceutical industry effluent; Ultrasound; Fenton; Hydrogen peroxide; Process intensification

**Howard Pike, Faisal Khan, Paul Amyotte. *Precautionary Principle (PP) versus As Low As Reasonably Practicable (ALARP): Which one to use and when. Pages 158-168.***

Safety and environmental risk go hand in hand with industrial development. However, it is unclear whether there is a linear or nonlinear relationship between risk and industrial development. Perhaps, it is case dependent. Some industrial endeavours such as offshore development, activities in a harsher environment, or development requiring new technologies (untested and untrusted technologies) may pose a higher risk (nonlinear) than more conventional industrial development activities (e.g., petroleum refineries, petrochemical plants, pipeline transportation, and the like). Public perception plays a critical role in defining the risk versus development relationship. The public perception of risk is dependent on awareness and understanding of potential hazards and their likelihood of occurrence, and most importantly, effective communication of these along with the associated uncertainty. Public awareness can have a profound effect on the development of public policy, which in many cases is driven more by perception rather than by sound science. This paper sheds light on this crucial issue. It investigates two commonly used concepts of policy and decision-making, the Precautionary Principle (PP) and As Low As Reasonably Practicable (ALARP). The paper provides a clearer understanding of both approaches with an illustrative example. It proposes a process to help readers understand where and when PP versus ALARP would be most applicable. The opinions and data presented here are based on the current study and relevant experience of the authors. The paper does not necessarily reflect the opinions of the authors' past or present employers nor correlate directly with previous projects on which the authors have worked.

- **Keywords:** As Low As Reasonably Practicable (ALARP); Precautionary Principle (PP); Safety decisions

**Fidel Ilizástigui Pérez. *Safety case process in Cuba: Transition from theory to practice.* Pages 169-176.**

Cuban Major Hazard/Safety Case regulations require that Facility Operators produce Operational Safety Cases with the aim of demonstrating that they can manage their risks of major accidents during facility operation to a level that is As Low as Reasonably Practicable (ALARP). The production of a good quality, fit-for-purpose Safety Case is a complex issue and must be cautiously approached by Facility Operators. Lessons from the Victoria Safety Case implementation and the Nimrod Review highlighted the need to ensure that a robust Safety Case process is in place before starting the work. This is of paramount importance in ensuring the process of production of the Operational Safety Cases delivers a final product – the documented Safety Case - that is Succinct, Home-grown, Accessible, Proportionate, Easy-to-understand and Document-lite (SHAPED). This paper provides insights into the manner in which the Safety Case production process is carried out by Facility Operators in accordance with a Safety Case Preparation Plan, which must previously be accepted by the Regulator. The Plan must be written in a way that defines the Safety Case process, emphasizes ownership and leadership of the process by the Facility Operator, maximizes workforce involvement in the production of the Safety Case deliverables and demonstrates and facilitates accessibility and usability of the final product – the documented Safety Case. The paper also provides information on the 'Pilot' Safety Case strategy which is a step-by-step, case-by-case process, currently being implemented by the Regulator, to lessen the burden of compliance with Safety Case requirements stated in the Regulations. According to this strategy, the entry of Major Hazard Facilities (MHFs) into the new regime will take place gradually and will not be linked to any specific licensing process.

- **Keywords:** Safety case regulations; Safety case process; Major hazard safety

**Silvia Patrícia B. Santana, Karla Patrícia Oliveira-Esquerre, Robson W. S. Pessoa, Brenner B. S. Silva. *Reliability of a collection and transport system for industrial waste water.* Pages 177-191.**

A safe operation of a wastewater collection and transport system must consider the probability of overflow events in and off the industry limits. In this paper the reliability of the collection and wastewater transport system of a refinery is assessed by using Cox reliability models. These models were adjusted to take into account the complex nature of the system. Rainfall is considered a model covariable since we are dealing with an open system. The probabilities of overflow from one retention tank either to another or to the water body were evaluated. The results indicate that through the creation of two scenarios, with different rainfall indices, in which it was possible to verify that the higher the index, the lower the reliability of the system. In conditions of rain, non-pumping, and in a one-day retention time, the reliability of the system did not exceed 76 % with a probability of overflow of 24 %. Nevertheless, after 4-day retention, the estimated reliability of the system dropped to 11.6 % and the probability of overflow increased to 88.4 %. And the system gets even more chaotic, if in the presence of rain, the activation of the pumps does not occur. The presence of rain is a factor that accelerates the occurrence of overflow.

- **Keywords:** Reliability analysis; Overflow; Industrial wastewater; Retention tanks; Cox regression model

**A.D. Ortiz-Marin, L.E. Amabilis-Sosa, E.R. Bandala, R.A. Guillén-Garcés, L.G. Treviño-Quintanilla, A. Roé-Sosa, G.E. Moeller-Chávez. *Using sequentially coupled UV/H2O2-biologic systems to treat industrial wastewater with high carbon and nitrogen contents.* Pages 192-199.**

This study evaluated the performance of a sequentially coupled UV/H<sub>2</sub>O<sub>2</sub>-anoxic system to treat industrial wastewater (IWW). Initial IWW characterization showed a high chemical oxygen demand (COD) load (13,261 mg L<sup>-1</sup>, 6,880 mg L<sup>-1</sup> of total organic carbon (TOC), 569 mg L<sup>-1</sup> of total nitrogen (TN), and an alkaline pH (9.1 ± 1.51). Using advanced oxidation processes (AOPs), removal efficiencies of 49.4 % of COD and 85 % of total organic carbon (TOC) were achieved after 60 min of UV-C irradiation (82 W m<sup>-2</sup>) using a H<sub>2</sub>O<sub>2</sub>/COD ratio of 0.78:1. Under these conditions, a 50 % transformation of TN into nitrites and nitrates (NO<sub>2</sub>+NO<sub>3</sub>)-N was also observed. After the AOP, the partially treated IWW was mixed with municipal wastewater (MWW) at ratio of 1:10, based on toxicity test results, and then used as the influent of the biological process. The biological process consisted of anoxic suspended and attached biomass coupled sequentially after the UV/H<sub>2</sub>O<sub>2</sub> system. Both biological systems (attached and suspended biomass reactors) efficiently removed (NO<sub>2</sub>+NO<sub>3</sub>)-N, achieving 85 % removal of TN, 41.8 % removal of TOC, and 49.2 % removal of COD and denitrification process was found to occur after the AOP through the biological systems. In addition, pH values ranging from 6 to 7.6 were observed after the biological treatment, which suggests that the resulting effluent could be treated using conventional water treatment.

- **Keywords:** Industrial wastewater; Anoxic systems; UV/H<sub>2</sub>O<sub>2</sub>; Nitrogen transformations

**Ammar Al Helal, Peter Milner, Ahmed Barifcani. *Oxygen scavenging performance of carboxylic acids formed during the degradation of monoethylene glycol regeneration products.* Pages 200-210.**

Previous studies have demonstrated that formic and glycolic acids could scavenge oxygen from aqueous solutions via complex radical mechanisms similar to that of erythorbic acid. Therefore, it is important to study the feasibility of using these common thermal degradation products obtained from the regeneration of monoethylene glycol (MEG). By replacing commercially used oxygen scavengers, such as sulfites, with these organic acids, the toxicity and subsequent environmental impact of oil and gas products could be easily reduced. Furthermore, these organic acids are rapid oxygen scavengers at low concentration, and they could be cost-effective; in addition, the chemical inventory could be reduced and project costs could be further optimized. The experimental results confirmed the potential of formic and glycolic acids to be used as oxygen scavengers downstream of the MEG regeneration process in the presence of manganese (II) ions as catalyst. Of the two commercial aqueous industrial oxygen scavengers tested, diethylhydroxylamine was an extremely rapid oxygen scavenger in salty aged lean MEG solutions under alkaline conditions, whereas methyl ethyl ketoxime exhibited extremely poor performance under similar conditions; therefore, it was ruled out as potential oxygen scavenger.

- **Keywords:** Salty aged lean MEG; Oxygen scavenger; Formic acid; Glycolic acid; DEHA; MEKO; Degraded MEG product; Natural gas processing

**Aynur Galeev, Yuri Chistov, Sergey Ponikarov. *Numerical analysis of flammable vapour cloud formation from gasoline pool.* Pages 211-222.**

In order to assess the potential hazard of oil and oil product spills, it is necessary to accurately determine the evaporation rate from the multi-component spill surface. In this paper, a multi-component pool evaporation model has been built and applied to the gasoline spill. The computational procedure has been implemented in the ANSYS Fluent code 18.0 through user-defined functions (UDFs). Gasoline is represented as a mixture consisting of a fixed number of individual components, and pseudo components (narrow boiling fractions). The model has been validated against the experimental data obtained in this study. The sensitivity analysis has been performed to assess the influence of wind velocity, pool thickness, and bund walls on the pool evaporation, the mass of vapour

within the flammability limits, and the size of the flammable cloud for hypothetical gasoline spills.

- **Keywords:** Gasoline; Pool evaporation; Vapour dispersion; Numerical simulation

**Mohammad Amin Mirrezaei, Ali Ahmadi Orkomi. *Gas flares contribution in total health risk assessment of BTEX in Asalouyeh, Iran. Pages 223-237.***

The health risk assessment of benzene, toluene, ethylbenzene and xylenes (BTEX) associated with the combustion of gas in gas flares of one of the largest gas refinery complex in Iran (South Pars gas complex in Asalouyeh, 1–10 phases) has been conducted based on Office of Environmental Health Hazard Assessment's (OEHHA) method. In this regard, AERMOD dispersion model coupled with WRF model has been used to predict the ground level concentration of pollutants emitted from gas flares. The accuracy of the dispersion model has been verified with measured ambient SO<sub>2</sub> data. The risk assessment results have shown that the chronic noncarcinogenic risk of BTEX emitted from gas flares is in the acceptable range in the residential area and most of refineries site. Regarding acute noncarcinogenic risk, the hazard indices (HIs) are only greater than one in refineries sites and are less than permitted level elsewhere in the study area. For carcinogenic risk, the cumulative risk of benzene and ethylbenzene are greater than 10<sup>-6</sup> in refineries sites and two cities (Asalouyeh and Nakhil Taghi), but in two camps nearby the gas flaring sites, the value is less than the allowable limit. Besides, the relative contribution of gas flaring in health risk assessment of BTEX is accomplished by calculating the health risk parameters with the measured BTEX concentrations at 10 receptors, which reveal the cumulative effects of all potential sources of BTEX throughout the study area. The comparison of health risk parameters has shown that the health risk of BTEX associated with flaring is in average 42 %, 2.6 % and 10.8 % of the overall health risk of BTEX in industrial areas, two cities and camps, respectively. It can be concluded that the contribution of gas flaring in industrial areas is noticeable and application of emission reduction policies at gas flaring, has a major effect on industrial areas and maybe has minor effects on the air quality of the residential areas.

- **Keywords:** Gas refinery; Cancer risk; Noncancer risk; AERMOD; WRF; Flaring

**Yimin Fan, Mengyu Lv, Xiaojun Niu, Jinling Ma, Dongqing Zhang. *The key step of gaseous phosphorus release in anaerobic digestion. Pages 238-245.***

Phosphine, a trace gas, is usually detected in aerobic digestion. To explore the key steps of gaseous phosphorus release during anaerobic digestion, a digestive medium was inoculated with anaerobic sludge and fertilizer to produce phosphine. The relationship between phosphine and digestive products, such as methane, hydrogen, carbon dioxide, and volatile fatty acids, was investigated. The experimental results indicated that methane and phosphine competed with each other for electron donors. Meanwhile, the concentration of phosphine reached approximately 110 mg/m<sup>3</sup> under methane production inhibition. Metabolite analysis indicated that fermentation of the butyric acid type favoured the production of phosphine, with a pH range of 6.3-7.0. The phosphine content was positively related to acetic acid and hydrogen, with correlation coefficients (R<sup>2</sup>) of 0.98 and 0.88, respectively. Molecular biology indicated that *Azotobacter*, *Dechloromonas*, and *Ruminococcaceae* were associated with phosphine production. To the best of our knowledge, this study is the first to explore the key step of gaseous phosphorus release in anaerobic digestion, providing a theoretical reference for phosphorus resource utilisation.

- **Keywords:** Phosphine; Anaerobic digestion; Methane; Hydrogen; Acetic acid

**Xiaojing Shi, Xiuyu Zhu, Xiaoxiao Zhao, Zhishan Zhang. *Performance evaluation of different extractive distillation processes for separating ethanol/tert-butanol/water mixture. Pages 246-260.***

In this study, a few extractive distillation processes with ethylene glycol as solvent are proposed to separate high-purity ethanol and tert-butanol from industrial effluents, including direct ED, indirect ED and heat pump assisted indirect ED. All these processes are optimized with targeting minimum annual total costs by a sequential iteration algorithm. After that, a head-to-head comparison is completed regarding distributions of cost, energy and CO<sub>2</sub> emission. The results showed that the direct ED is the most economical process reducing minimum annual total costs by 30.15 % than the heat-pump assisted indirect ED, while the latter is the most energy-efficient process saving energy consumption and CO<sub>2</sub> emissions by 14.78 % and 21.79 % than the direct ED.

- **Keywords:** Extractive distillation; Optimization; Heat pump; Energy saving; Ethanol/tert-butanol/water

**Mansour Sarafraz, Morteza Sadeghi, Ahmadreza Yazdanbakhsh, Mostafa M. Amini, Mohsen Sadani, Akbar Eslami. *Enhanced photocatalytic degradation of ciprofloxacin by black Ti<sub>3+</sub>/N-TiO<sub>2</sub> under visible LED light irradiation: Kinetic, energy consumption, degradation pathway, and toxicity assessment. Pages 261-272.***

In this work, the photocatalytic degradation of ciprofloxacin (CIP) by black Ti<sub>3+</sub>/N-TiO<sub>2</sub> under visible LED light irradiation (b-N-TiO<sub>2</sub>/LED) was studied for the first time. Characterization of the prepared photocatalyst was performed by XRD, UV-Vis DRS, FE-SEM, EDS, HRTEM, and BET techniques. The b-N-TiO<sub>2</sub> nanoparticles with high surface area of near 100 m<sup>2</sup> g<sup>-1</sup> and narrow band gap of 2.0 eV, exhibited a remarkable photocatalytic performance on the degradation (100 %) and mineralization (82 %) of CIP under visible LED light irradiation. The maximum degradation was found at reaction time = 70 min, initial CIP concentration = 0.5 mg L<sup>-1</sup>, pH = 6.7, and catalyst dosage = 0.43 g L<sup>-1</sup>. Based on the results, both the hole (h<sup>+</sup>) and hydroxyl radical (OH) played a major role than the superoxide radical (O<sub>2</sub><sup>-</sup>) in CIP degradation. Although common coexisting anions in water had a slight negative effect on CIP degradation; humic acid (HA), especially in higher amounts, showed a considerable inhibitory effect on degradation process. Besides, the intermediates of CIP degradation were ultimately transformed into simple compounds. Accordingly, toxicity assessments revealed that the treatment of CIP solution by b-N-TiO<sub>2</sub>/LED process remarkably resulted in diminished toxicity compared to the untreated controls. The energy utilized in this study was far less than that used in other studies. Moreover, we found that b-N-TiO<sub>2</sub> had desirable stability and can be reused for more than five runs of experiments. Collectively, based on our findings, the b-N-TiO<sub>2</sub>/LED process is a promising, low cost and feasible candidate can be used for degradation and mineralization of antibiotics like CIP in real water samples.

- **Keywords:** Ciprofloxacin; Black Ti<sub>3+</sub>/N-TiO<sub>2</sub>; Photocatalytic degradation; Visible LED; Mineralization; Reusability

**Saeed Soltanali, Maryam Mashayekhi, Seyed Reza Seif Mohaddecy. *Comprehensive investigation of the effect of adding phosphorus and/or boron to NiMo/γ-Al<sub>2</sub>O<sub>3</sub> catalyst in diesel fuel hydrotreating. Pages 273-281.***

In order to comprehensively investigate the effect of boron (B) and phosphorous (P) promoters on the catalytic performance of a hydrodesulfurization catalyst (NiMo/γ-Al<sub>2</sub>O<sub>3</sub>, separate or simultaneous addition of the two promoters and the method of their addition to the catalyst solution or support have been studied by physical, chemical and reactor

evaluation of nine synthetic catalysts using a diesel fuel feed containing 11,500 ppm of sulfur and 250 ppm of nitrogen. For better evaluation of the synthetic catalysts, their surface area, morphology, crystalline structure, regeneration temperature and acidity have been studied by ICP, XRD, Raman, FTIR, TPR, BET, FESEM and TPD analyses. Reactor evaluations have been performed at a temperature of 340 °C, pressure of 65 bar, LHSV of 0.8 h<sup>-1</sup> and hydrogen to hydrocarbon ratio of 250 and the amounts of sulfur and nitrogen resulting from each catalyst have been determined. The catalysts showed very different performances in the absence or presence of P and B promoters in the desulfurization and hydrodenitrogenation processes. The presence of P and B promoters seems to be necessary in the hydrodesulfurization process. However, the presence of P and B promoters in the HDN process depends on the type and method of the promoter addition.

- **Keywords:** Hydrodesulfurization; Hydrodenitrogenation; Diesel fuel; Boron; Phosphorus; NiMo/γ-Al<sub>2</sub>O<sub>3</sub>

**Zhi Wang, Duanlin Cao, Zishuai Xu, Jianlong Wang, Lizhen Chen. *Thermal safety study on the synthesis of HMX by nitrourea method*. Pages 282-288.**

HMX is one of the best high-energy explosives in military applications. In this paper, the reaction calorimeter (RC1e) was used to monitor the reaction process of HMX synthesis by the nitrourea method. The research results show that the heat release rate is large on the reaction feeding stage, the feed rate should be controlled. The thermal parameters, such as adiabatic temperature rise ( $\Delta T_{ad,r}$ ) and maximum temperature of the synthesis reaction (M<sub>TSR</sub>), were calculated for assessing the thermal hazard of HMX synthesis. Although the urea nitrification stage is safer, the operating conditions of other reaction processes also need to be redesigned to improve the process safety level. These studies have potential applications in inherently safer operating measures and safer storage and transportation.

- **Keywords:** Maximum temperature of the synthesis reaction; Thermal characteristics; Exothermic curves

**Wei Pan, Huimin Jin, Zhengzhou Liu, Jiahui Tang, Shuangyi Cheng. *Experimental and theoretical study on strengthening leaching of sulfide ores by surfactants*. Pages 289-299.**

The purpose of this research was threefold: to change the surface tension of an ore-leaching solution through adding surfactants, to improve the bioleaching of sulfide ore, and to strengthen the desulfurization effect of microorganisms on sulfide ore. Taking different types of surfactants in various concentrations as the impact factors, we evaluated their effect on the relationship between the change rate of surface tension, the attenuation coefficient of the surfactants, and the ore surface desulfurization rate. The experimental results indicate that when surfactants of different types and of different concentrations are added to an ore-leaching solution, they can change the solution's surface tension by different degrees and can influence the effects of bacterial desulfurization. The experimental combination with the highest surface desulfurization rate had a dosage of bacterial agent (*Thiobacillus acidophilus*) of 40 mL, a desulfurization treatment time of 5 days, and a surfactant (Tween80) concentration of 0.1 %-a combination that achieved 31.68 % desulfurization. By this method, we effectively promoted the desulfurization effect of *Thiobacillus acidophilus* on sulfide ore and ultimately improved the leaching effect. We then used the best surfactant as the leaching aid in subsequent experiments on microbial leaching desulfurization. A three-dimensional reconstruction of the temperature field of an ore heap was conducted by simulating the dynamic self-heating process of the ore heap. The final results showed that the self-heating of the sulfide ore heap that we treated by desulfurizing bacteria was hindered to

some extent, and therefore the goal of preventing the spontaneous combustion of sulfide ore was achieved.

- **Keywords:** Surfactant; Sulfide ore; Enhanced leaching; Surface desulfurization rate; Three-dimensional reconstruction of temperature field

**Humair Ahmed Baloch, M.T.H. Siddiqui, Sabzoi Nizamuddin, N.M. Mubarak, Mohammad Khalid, M.P. Srinivasan, G.J. Griffin. *Solvothermal co-liquefaction of sugarcane bagasse and polyethylene under sub-supercritical conditions: Optimization of process parameters. Pages 300-311.***

The co-liquefaction of mixtures of sugarcane bagasse and high density polyethylene (HDPE) in ethanol under subcritical and super-critical conditions was studied with the objective of finding optimal process conditions for bio-oil yield and overall conversion. Taguchi method was employed to design with 9 experiments to find the effect of 4 independent variables (temperature, reaction time, biomass to plastic composition and solvent-to-biomass ratio) on the co-liquefaction of plastic and biomass for total conversion and bio-oil yield. The optimal results showed 60 % conversion with bio-oil yield 32.3 % having HHV of bio-oil 29.6MJ/kg respectively. The predicted model indicated a good fit with that of experimental data. Furthermore, detailed characterizations of bio-oils were carried out such as higher heating value (HHV), chemical composition, NMR analysis, elemental analysis, FTIR and thermogravimetric analysis. The co-liquefaction of sugarcane bagasse and polyethylene was found effective to improve the qualitative and quantitative features of products from the biomass.

- **Keywords:** Co-liquefaction; High density polyethylene; Sub/super critical fluid; Optimization; Waste plastics

**Wei Jen Lok, Lik Yin Ng, Viknesh Andiappan. *Optimal decision-making for combined heat and power operations: A fuzzy optimisation approach considering system flexibility, environmental emissions, start-up and shutdown costs. Pages 312-327.***

Variations in energy demands require combined heat and power (CHP) systems to be more flexible in adjusting its operations. However, high flexibility is often achieved at the expense of other aspects. In other words, increasing flexibility of a CHP system would require large number of equipment to start-up or shutdown. This would lead to potentially high emissions and high start-up/shutdown costs due to sub-optimal fuel choices and poor selection of technologies respectively. In this respect, it would be challenging to determine the optimal CHP operation with high flexibility, low emissions and low start-up/shutdown costs. To address this challenge, operational optimisation must be considered. In this paper, a multi-objective fuzzy optimisation model was developed to optimise system flexibility, fuel emissions, equipment start-up and shutdown costs for a CHP system operation to meet varying energy production requirements. Essentially, fuzzy optimisation is used to maximise the degree of satisfaction among the three mentioned objectives. To demonstrate the proposed approach, a multi-fuel CHP case study consisting of several scenarios was solved. Results from the case study show that a trade-off CHP operation was determined for increased production. The trade-off operation had the degree of satisfaction of 35 % for each objective. The obtained degree of satisfaction indicates that a balance between flexibility, emissions and costs was achieved. In addition, chosen technologies and fuels were analysed and classified under categories such as "must have", "optional" and "must avoid".

- **Keywords:** Combined heat and power; Fuzzy optimisation; Start-up and shutdown costs; Emissions; System flexibility

**Wen Fu, Ke Zhang, Jiangtao Wu. *Flammability limits of benzene, toluene, xylenes from 373 K to 473 K and flame-retardant effect of steam on benzene series. Pages 328-339.***

Typical benzene series (benzene, toluene, xylenes), while having important applications in chemical industry, are also threatening industrial safety and daily life due to high flammability. In this work, we measured the flammability limits of benzene, toluene, xylenes by ASHRAE method based on E681-09 at elevated temperatures (373 K, 423 K and 473 K). As the temperature increased, the flammable concentration ranges of benzene series expanded. On the basis of flammability limits experimental results, the flame-retardant effect of steam (H<sub>2</sub>O) on benzene, toluene, o-xylene, m-xylene, and p-xylene were investigated at 423 K separately. These experimental data were correlated with the extended Le Chatelier's law and compared with theoretical estimations based on adiabatic flame temperature (AFT) method. The experimental results were completely reproduced by the extended Le Chatelier's law. The lower and upper flammability limits (LFLs and UFLs) of benzene/toluene + H<sub>2</sub>O agreed well with the estimations, and the upper flammability limits of xylenes + H<sub>2</sub>O were within acceptable absolute deviation range. The average absolute deviations (AADs) of the lower and upper flammability limits for benzene series + steam between experimental results and optimized estimations were 0.07 % and 0.38 % separately. Moreover, flame-retardant effect of other diluents (N<sub>2</sub> and CO<sub>2</sub>) on benzene series were calculated theoretically, and all the critical flammable ratios (CFRs) were close to 1. The results showed that the flame retardancy on benzene series need to be considered seriously rather than using common diluents.

- **Keywords:** Flammability limits; Flame-retardant effect; Benzene series; Diluents; Theoretical estimation

**Pengfei Wang, Han Han, Ronghua Liu, Runze Gao, Gaogao Wu. *Effect of outlet diameter on atomization characteristics and dust reduction performance of X-swirl pressure nozzle. Pages 340-351.***

In this study, experimental studies on the atomization characteristics and dust reduction performance of six different X-swirl nozzles with different outlet diameters were performed. The results of the nozzle atomization characteristics shows that, as the diameter of the nozzle increased, the flow rate of the nozzle gradually increased, while the flow coefficient kept decreasing almost linearly. Meanwhile, with the increase of the outlet diameter, the nozzle range and droplet velocity decreased continuously, while atomization angle and droplet size exhibited an increasing trend in general. From results of the dust-reduction experiment, considering the dust-reduction efficiency and water consumption, it is more appropriate to select a nozzle with an outlet diameter of 1.2 mm when the water supply pressure is higher than 4.0 MPa. When the water supply pressure was low, as the diameter of the outlet increased, the dust-reduction efficiencies of the nozzle for both the total dust and the respirable dust increased significantly. Therefore, under low water supply pressure, when the water consumption at the engineering application site is not limited, using a nozzle with a larger outlet diameter can achieve higher dust-reduction efficiency.

- **Keywords:** X-swirl pressure nozzle; Atomization characteristics; Dust reduction performance; Outlet diameter; Dust

**Zahra Naghavi-Konjin, Seyed-Bagher Mortazavi, Hassan Asilian-Mahabadi, Ebrahim Hajizadeh. *Ranking the occupational incident***

***contributory factors: A Bayesian network model for the petroleum industry. Pages 352-357.***

**Introduction:** A vast amount of research has been conducted to identify human and organizational factors that contribute to the occurrence of occupational incidents. Considering the identified factors, the question is how much the occupational incident probability will decrease in the absence of one or more recognized contributory factors.

**Methods:** Twenty-one fatal accident reports were selected for Root Cause Analysis (RCA). The contributory factors were identified by content analysis of the accident scenarios. A 5-point Likert questionnaire was developed to measure the probability of identified factors. Using the identified contributory factors and their corresponding probabilities, a Bayesian network model was constructed for estimating the probability of the occupational incident in the absence of each contributory factor.

**Results:** Procedure violation, poor risk perception, and poor management commitment were three top-ranking contributory factors. The Bayesian network estimated that preventing procedures violation could cause a reduction of 44 % in the occupational incident probability.

**Conclusion:** Using Bayesian network's advantages is an effective technique for quantifying occupational safety risks. Ranking the contributory factors enables us to choose the most effective prevention strategies. Procedure violation (a type of unsafe act) was the most influencing factor in occupational incident probability.

- **Keywords:** Occupational incident; Contributory factor; Bayesian network; Petroleum industry

***Gabriel Pérez-Lucas, Marina Aliste, Nuria Vela, Isabel Garrido, José Fenoll, Simón Navarro. Decline of fluroxypyr and triclopyr residues from pure, drinking and leaching water by photo-assisted peroxonation. Pages 358-365.***

Groundwater is a source for drinking water in many countries, and its use is seriously threatened by the leaching of agrochemicals through the soil. With this aim, the oxidation of triclopyr and fluroxypyr in water was investigated at lab-scale using heterogeneous photocatalysis and photo-assisted ozonation combined with hydrogen peroxide H<sub>2</sub>O<sub>2</sub> (peroxone process). For both herbicides, the order of effectiveness of the photo-assisted treatments in pure water were as follows: O<sub>3</sub>/H<sub>2</sub>O<sub>2</sub>>ZnO/Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub>>TiO<sub>2</sub>/Na<sub>2</sub>S<sub>2</sub>O<sub>8</sub>. Comparing the three types of water, the rate constants through peroxone/UV process were in the order: Pure>Drinking>Leaching water, according to the complexity of the matrix. After two hours of treatment, fluroxypyr was completely removed from pure water, while 90 % and 55 % of its initial mass were removed from drinking and leaching water, respectively. On the other hand, the degradation of triclopyr was significantly slower. In this case, after two hours of illumination the complete degradation was not reached in any case. Owing to the generation of hydroxyl radicals (HO) the water treatment with O<sub>3</sub>/H<sub>2</sub>O<sub>2</sub>/UV can be considered as an eco-friendly technology, although the substances present in the matrix, mainly in leaching water, can scavenge HO decreasing the photooxidation rate of both herbicides.

- **Keywords:** Herbicides; Heterogeneous photocatalysis; Peroxonation; Water