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Jianjun Cai, Ronghua Zeng, Wenheng Zheng, Shubin Wang, Jie Han, Kaiqiang Li, Ming Luo, Xingying Tang. *Synergistic effects of co-gasification of municipal solid waste and biomass in fixed-bed gasifier*. Pages 1-12.

The co-gasification of refuse derived fuel (RDF) and biomass is a promising technology for environmentally friendly municipal solid waste (MSW) utilization. Herein, we investigated the co-gasification of RDF and straw mixtures. The development of syngas suggested that higher temperature and equivalence ratio (ER) values promote syngas yield during gasification and co-gasification. Temperature plays a positive key role in gas yield and carbon conversion efficiency once the ER is higher than 0.3 during co-gasification. Except for an ER of 0.3, synergistic enhancements in carbon conversion efficiency, gas yield, and cold gas efficiency were observed for co-gasification. The positive synergistic effects of co-gasification mainly appeared in lower ER (0.1−0.2) and higher temperatures (800−900°C); however, the negative synergistic effects more tend to appear in higher ER (0.3−0.4). From the development of bottom ash in co-gasification, at higher temperature and ER values, potassium in the bottom ash was favored to stay in sulfur-containing compounds; whereas at lower temperature and ER values, potassium preferred to exist in potassium chloride. A higher calcium content more easily enriched in small particles that were integrated into aluminosilicate led to the formation of sticking ash particles, which could promote significant melting agglomeration. However, these melting agglomerations could be suppressed by adding straw into the RDF. These results provide a feasible method for the resource utilization of MSW.

- **Keywords:** Municipal solid waste; Biomass; Gasification; Syngas; Synergistic enhancement

Horng-Jang Liaw, Yuan-Ruei Liou. *Systematic thermal and flammability hazard analysis of a DMPAT explosion accident in Taiwan*. Pages 20-33.

In 2016, a serious accident involving a thermal explosion of o,o-dimethyl phosphoramidothioate (DMPAT) resulted in the death of one operator and the serious injury of another at a pesticide plant in Taichung, Taiwan. This study conducts a systematic thermal and flammability hazard analysis of DMPAT in order to better understand the decomposition and reaction events that led to the explosion. The temperature and pressure behavior of DMPAT were analyzed using a PHI-TEC II adiabatic calorimeter, while the thermal stability was investigated using a thermogravimetric

analyzer/differential scanning calorimeter (TGA/DSC). The liquid and solid samples formed during the test and heating process were analyzed using attenuated total reflectance (ATR), while the gas phase compounds were examined by TGA-FTIR and pyrolysis-gas chromatography-mass spectrometry (Py-GC/MS). The results indicate that, during the explosion, the vapors of DMPAT and its impurities partially oxidized in air and the resulting heat of the reaction elevated the temperature of the liquid DMPAT at the vapor liquid interface, which resulted in temperatures higher than the onset decomposition temperature. A significant decomposition of DMPAT then occurred, which released more heat and this brought about the decomposition of the remaining DMPAT. The result was a further rapid rise in the system temperature until the point where a thermal explosion occurred. This study gave evidence that combustion of decomposition products may occur alongside a thermal explosion of the main reactive material if the final temperature of the decomposition reaction exceeds the auto-ignition temperatures of the decomposition products, and sufficient air is available.

- **Keywords:** o,o-dimethyl phosphoramidothioate (DMPAT); Accident; Incident investigation; Decomposition; Thermal hazard

K. Tajziehchi, S.M. Sadrameli. *Optimization for free glycerol, diglyceride, and triglyceride reduction in biodiesel using ultrafiltration polymeric membrane: Effect of process parameters*. Pages 34-46.

Membrane purification technique as an environmental-friendly process to the conventional biodiesel water washing should not only achieve high purified biodiesel but also should be feasible from an economic perspective. Consequently, a better comprehension of the process parameters on different impurities is a vital requirement for optimizing the membrane separation process for biodiesel purification. To achieve this aim, commercial PolyVinyliDene Fluoride (PVDF) membrane with 100 kDa molecular weight cut-off was used for the ultrafiltration of crude biodiesel. Response surface methodology (RSM) was applied to study the impact of process variables including temperature, transmembrane pressure, and water addition on free glycerol, diglyceride, and triglyceride reduction as well as permeate flux as responses. Simultaneous reduction of mentioned impurities to the limits imposed by international standards achieved at pressures lower than 2 bars and temperatures lower than 30 °C with a low permeate flux of 20 kg/m2.hr. This low permeate flux can be an obstacle to the commercial consumption of biodiesel. This low permeate flux is due to the limitation of triglyceride impurity in the biodiesel imposed by EN 14214 standards.

- **Keywords:** Biodiesel purification; Linseed oil; Ultrafiltration; Polymeric membrane; Process optimization

André Laurent, Alexis Pey, Peter Gurtel, Bruno Fabiano. *A critical perspective on the implementation of the EU Council Seveso Directives in France, Germany, Italy and Spain*. Pages 47-74.

From 1982–2012, an important legislation, known as Seveso Directives I-II-III and amendments, was adopted in the European Union to regulate and prevent major industrial accident hazards. This European legislation was transposed, applied and implemented in each European Member State and after nearly forty years it is worthwhile to look back and also to look forward to key issues relevant to actual Seveso implementation. Authors of this paper are all members (retired or active) of the Loss Prevention Working Party of the European Federation of Chemical Engineering, which started in 1971. This article examines and compares, for the four EU Member States France, Germany, Italy and Spain, the structures and practices for the implementing of the European rules. Difficulties, variations in application and the quality of enforcement of this complex process are critically discussed, including proper analysis of worked

examples. Finally, a particular attention is paid to the different ways in which the control and inspection practices of each of the Member States concerned are implemented.

- **Keywords:** Seveso legislation; Implementation; Inspection practices; LUP criteria

Qi Jing, Dan Wang, Qingming Liu, Xu Chen, Yang Shen, Zhisong Wang, Yingpeng Zhong. *Inhibition effect and mechanism of ultra-fine water mist on CH4/air detonation: Quantitative research based on CFD technology*. Pages 75-92.

As an effective depressant, ultra-fine water mist has broad application prospects in reducing the loss caused by a gas detonation. Ultra-fine water mist can be sprayed into coal mine roadways or natural gas pipelines when detecting the radiation spectrum signal of the explosion, to prevent further expansion of the explosion. A two-dimensional pipeline model was designed to study the effect and mechanism of methane detonation suppression by monodisperse ultra-fine water mist with a diameter of 10 μm. The methane detonation at the stoichiometric concentration (9.5 %) will decay to a deflagration under the suppression of fine water mist of 160 g/m3. When the concentration of fine water mist is less than 160 g/m3, the detonation wave has a slight attenuation in the water mist area, while it returns to a stable detonation state after passing through the mist area. The results also indicate that a water mist above 800 g/m3 can effectively suppress detonation and eventually lead to flame extinguishment. The critical transition concentration of ultra-fine water mist that can decay a methane detonation to a deflagration and the critical extinction concentration of ultra-fine water mist that completely suppresses a detonation within the explosion limit were obtained, providing a visual reference for the suppression of methane explosion accidents in coal mine tunnels or pipelines.

- **Keywords:** Detonation suppression; Explosive mode; Critical concentration; Numerical simulation

Yujie Lin, Longhua Hu, Xiaolei Zhang, Yuhang Chen. *Experimental study of pool fire behaviors with nearby inclined surface under cross flow*. Pages 93-103.

Few studies have been done on the flame behavior of pool fires, as a typical fire incident in process industry, with a nearby inclined surface, i.e., in hilly area or with obstacle. This work studied the influence of the nearby inclined surface on flame height and air entrainment of pool fires in still air and under cross flow with various pool sizes and regression rates. The inclined angles of the nearby surface were 0°, 20°, 30° and 40° from horizontal direction and cross flow speed ranged within 0−3 m/s. Experimental results show that the flame height increases with increasing inclined angle of nearby surface. Fire Dynamics Simulator (FDS) was adopt to interpret the air entrainment flow field. The nearby inclined surface restricts air entrainment and introduces a negative pressure zone in the upwind part and stretches the flame along the nearby inclined surface. Cross flow supplies additional air while enhancing the negative pressure. Formulas are proposed based on overall buoyancy led by pool fire, cross flow momentum and a deduced characteristic global nearby inclined surface factor, showing good correlation with the experimental results.

- **Keywords:** Pool fire; Cross flow; Nearby inclined surface; Flame behavior

Uthradevi Kannan, Sabumon P.C., Shihabudheen M. Maliyekkal. *Development of an eco-friendly and reusable point-of-use disinfection system*. Pages 104-113.

The nanoscale silver-based disinfection of water is a proven technology. However, the lack of an affordable and easy-to-use system for controlled and sustained release of silver ions into the water has hindered its mass deployment in the field. The present work addresses this critical issue by developing a film-forming composite that can release silver ions at a controlled and sustained rate. The paper also demonstrates the application of the composite film to disinfect water taking Escherichia coli MTCC 443 as the model microorganism. The composite is fabricated by eco-friendly materials such as chitosan, reduced graphene oxide, silver nanoparticles, and tannic acid as feedstock. The hydraulically stable composite can either be used as a stand-alone antibacterial strip or can be coated on a suitable solid surface such as a mud-pot, sand particles or a specially designed reactor to create a point-of-use disinfection system. The composite film is reusable and can consistently produce 3 log reduction of microbes over several cycles. The conservative estimates show that the technology can provide microbial free water at the cost of < 0.5 USD per 1000 L. The composite may find applications in rural areas and urban slums where access to treated water is limited.

- **Keywords:** Nanocomposite; Silver nanoparticles; Water purification; Point-of-use disinfection system; Sustainable materials

Kazem Godini, Ghasem Azarian, Alireza Kimiaei, Elena Niculina Dragoi, Silvia Curteanu. *Modeling of a real industrial wastewater treatment plant based on aerated lagoon using a neuro-evolutive technique*. Pages 114-124.

Aerated lagoons are biological systems used for the treatment of different types of wastewaters and many operating parameters influence the performance of these systems. Thus, in the current study, an industrial aerated lagoon system was modeled in terms of the operating parameters with the goal of predicting its performances under different operating conditions in order to highlight possible bottlenecks or potential improvements. For this purpose, a neuro-evolutive approach, combining differential evolution (DE) algorithm and artificial neural networks (ANN), was employed. Two DE variants based on opposition-based learning and of chaos theory were used to determine the optimal models and to perform a process optimization. Multiple models in various configurations (simple or organized in stacks, with single or multiple outputs) were determined. The mean squared error of the best solutions were in the order of 10−4, illustrating a good agreement between the model predictions and experimental data and demonstrating the effectiveness and reliability of the developed models.

- **Keywords:** Aerated lagoons; Wastewater treatment; Artificial neural networks; Differential evolution algorithm; Modeling; Optimization

Jude O. Ejeh, Songsong Liu, Lazaros G. Papageorgiou. *An MILP model for safe multi-floor process plant layout using the domino hazard index*. Pages 137-165.

In this paper, an optimisation-based approach to obtain safe multi-floor process plant layout designs using the domino hazard index (a sub-index of the integrated inherent safety index) is presented. A mixed integer linear programming (MILP) model is proposed to obtain the economically optimal multi-floor layout design considering connection by pipes, horizontal and vertical pumping of process fluids, purchase of land, fixed and area-dependent construction of floors, the financial risk associated with hazardous events and their escalation potential, and the installation of passive protection devices. Hazardous events such as pool fires, jet fires, flash fires, fireballs and blast waves resulting from explosions are considered using a novel and more realistic estimation of safety distances between equipment items. A bi-objective optimisation problem is also considered, minimising the layout costs and the total domino hazard index values for the plant,

adopting the ϵ-constraint method. The proposed model is then applied to an 11-unit case study susceptible to each of these hazardous events, obtaining results with the optimal layout and protection device configurations in a relatively short amount of time.

- **Keywords:** Multi-floor process plant layout; Mixed integer linear programming (MILP); Multi-objective optimisation; Domino hazard index; Safety

Yihuan Wang, Peng Zhang, Guojin Qin. *Reliability assessment of pitting corrosion of pipeline under spatiotemporal earthquake including spatial-dependent corrosion growth*. Pages 166-178.

The pitting corrosion of pipelines subjected to the spatio-temporal earthquake was evaluated to illustrate the failure probability of multiple loading conditions. The pipeline vibration was modeled as a coupled 3D vibration equation considering the uncertain soil parameters. Using a combination of the Gamma process and Gaussian copula function implemented time-dependent corroded growth of single defect as well as the spatial-dependent between corroded depth growths of different defects. All modeling was embedded in a frame of Bayesian inference and Markov chain Monte Carlo (MCMC) simulation techniques to predict the future corroded growth by reported in-line inspections (ILIs). Moreover, the Monte Carlo simulation (MC) technique was used to evaluate the reliability of the pipeline system, including multiple corroded defects. A case study was employed to prove the application of all proposed models. The results indicate that the reliability analysis of pipelines under the earthquake considering pitting corrosion growth is of considerable significance to the accuracy of the evaluation, which can inform operators from process industry to mitigate the risk of pipeline failure.

- **Keywords:** Coupled vibration; Pitting corrosion; Spatiotemporal earthquake; Uncertainty parameters; In-line inspections

Grzegorz Poplewski, Dominic C.Y. Foo. *An extended corner point method for the synthesis of flexible water network*. Pages 210-224.

This paper presents an extended methodology for the design of flexible water network (FWN). In many water network systems, parameters of the water-using processes (e.g. flow rate, concentration, etc.) vary due to operational changes. Hence, it is important to synthesize a FWN that can absorb these changes, so to ensure business sustainability. In this paper, the recently established corner point method for FWN synthesis is extended to cater the discrete way of process parameters change. The newly proposed methodology ensures the synthesized FWN to achieve the intended objective, i.e. minimum fresh water intake and minimum total pipeline length, while satisfying the various process constraints (e.g. flow rate, concentration, etc.). To address the multiple-objective problem, a three-step optimization method has been developed. The corner point method is also extended to synthesize a FWN that achieves the minimum total annualized costs (TAC). A literature case study was used to show the usefulness of the proposed method.

- **Keywords:** Process integration; Water minimization; Mathematical programming; Process changes; Flexible design

Andrea P. Ortiz-Espinoza, Arturo Jiménez-Gutiérrez, Mahmoud M. El-Halwagi, Nikolaos K. Kazantzis, Vasiliki Kazantzi. *Comparison of safety indexes for chemical processes under uncertainty*. Pages 225-236.

The fatal consequences of industrial incidents have made evident the need for suitable tools to develop inherently safer process design options. Traditionally, in a process design project, the evaluation of safety aspects is left for analysis after the detailed design has been completed. This approach leads to the use of control loops, barriers and protection

layers as the only ways to prevent incidents and to reduce the possible outcomes. An alternative to this approach is the application of the concept of inherent safety, which was introduced to set up several principles that aim to enhance process safety by eliminating, avoiding or minimizing sources of risk. In this work, we present a comparison of different safety metrics in their role to evaluate the risk associated with a given process design. The indices selected for consideration are the Dow's fire and explosion index (F&EI), the fire and explosion damage index (FEDI), the process route index (PRI) and the process stream index (PSI). All these indices use different input information and their outcomes have different rankings. The metrics were applied to an ethylene production process from shale gas to identify hazard levels, and the location of streams and pieces of equipment that pose the highest hazard within the process. An evaluation of the indices in their capability to track design changes in operating conditions aiming to improve the safety level of the process was developed. To perform the assessment of the safety metrics in a more extensive manner, an uncertainty analysis based on a Monte Carlo simulation framework was implemented and compared to the traditional use of single-value design variables. Within this context, an insightful assessment of uncertainty's effect on process safety characteristics was achieved because of the identification of ranges of safety-relevant performance outcomes (zones of risks and opportunities) that can be probabilistically characterized. The application of the approach to the ethylene process showed how some indexes are better suited to capture the hazard characteristics associated with the process when changes in the operating conditions of most hazardous section were implemented. The methodology can be extended to other processes of interest, and may serve as a basis for the safety and process design community to propose adjustments in the structure of safety indices based on a better understanding of their performance and reliability as part of broader efforts towards their continuous improvement and refinement.

- **Keywords:** Process safety; Inherent safety; Uncertainty analysis; Monte Carlo simulations; Ethylene production

Malihe Barahoei, Mohammad Sadegh Hatamipour, Saeed Afsharzadeh. *Direct brackish water desalination using Chlorella vulgaris microalgae*. Pages 237-248.

The objective of this study was to investigate the suitability of direct use of Chlorella vulgaris for brackish water desalination as a new conceptual technique. First, the adaptation of Chlorella vulgaris in saline water was performed, and then the living microalgae cells were utilized for the desalination process using a bubble column photobioreactor. The effect of culture medium, time, salinity and initial inoculum on the microalgae growth and salinity removal was investigated and the optimum conditions were obtained by RSM−CCD method. To assure the consumption of sodium chloride (NaCl) content of water by microalgae, the BG11 culture medium was modified by substituting its chloride and sodium containing salts by nitrate, calcium and potassium containing minerals. The results indicated that the enhancement of microalgae growth and salt removal efficiency were more pronounced in the modified-BG11 (MBG11) culture medium. Using Chlorella vulgaris microalgae in the MBG11 culture medium, the decrease in brackish water electrical conductivity for different NaCl concentrations between 1000 and 5000 ppm, was between 80 % and 40 %, respectively. Atomic absorption and flame photometry analyses confirm the hypothesis of adsorption of Na+ ions on the Chlorella vulgaris cell surface.

- **Keywords:** Desalination; Microalgae; Bubble column photobioreactor; Chlorella vulgaris; BG11 culture medium

Somdipta Bagchi, Manaswini Behera. *Methanogenesis suppression and increased power generation in microbial fuel cell during treatment of chloroform containing wastewater*. Pages 249-255.

Chloroform is a commonly found solvent in industrial wastewater and is very toxic if present in high concentration. Chloroform degradation in anaerobic processes has been reported earlier and it has also been used as a methanogenesis suppressor in rumen and rice fields. Methanogenesis is undesirable in a microbial fuel cell (MFC) operation, as it results in substrate competition between methanogens and exoelectrogens, thereby reducing the electricity output. Hence, an attempt has been made in this research work to study the effect of chloroform on the performance of MFCs and its effectiveness as methanogenesis suppressor. MFCs with different chloroform dosages in batch as well as continuous mode (0 mM, 8 mM, 16 mM and 22 mM; 0 mM and 22 mM) were operated. High open circuit voltages in batch MFC22 (781 mV) and 53 % higher peak power densities in dosed continuous MFC confirmed its efficiency as a methanogenesis suppressor. Further experimentations showed 74 % lower internal resistance in dosed MFCs. Higher coulombic efficiencies of 31.2 % (MFC22) and 18 % (MFCC22) were noted in dosed reactors than the control reactors (MFC0 – 23.8 % and MFCC0 - 8%). At the end of batches, chloroform concentration was found to be negligible, confirming its degradation in MFC.

- **Keywords:** Chloroform; Methanogenic suppression; Coulombic efficiency; Power density; Microbial fuel cell

Anna Crivellari, Sarah Bonvicini, Alessandro Tugnoli, Valerio Cozzani. *Multi-target Inherent Safety Indices for the Early Design of Offshore Oil&Gas Facilities*. Pages 256-272.

Improved tools are needed to manage major accident hazard of progressively more complex offshore oil&gas systems in environmentally sensitive areas. Inherent safety principles provide a strategic opportunity to reduce major accident hazards since the early design phase, but a suitable metric to orient safer design choices is needed to apply such principles intro practice. This study aims at providing a systematic approach to the assessment of the hazard profile of alternative process designs in offshore oil & gas production facilities. A novel methodology providing a ranking of inherently safer solutions in conceptual design is described. The methodology is able to highlight the different contributors to the safety profile of the offshore oil & gas production system, linking them to the specific features of the design. The proposed approach, based on multi-criteria Key Performance Indicators (KPIs), addresses different targets (people, assets, environment) and provides a quantitative assessment of the safety score, accounting for both the possible accident consequences and their credibility. An application to a case study concerning an offshore facility for gas production is discussed to demonstrate the potential of the methodology.

- **Keywords:** Inherently safer design; Key performance indicators; Oil&Gas operations; Offshore installations; Process safety; Major accident hazard

Ammar H. Elsheikh, Vikrant P. Katekar, Otto L. Muskens, Sandip S. Deshmukh, Mohamed Abd Elaziz, Sherif M. Dabour. *Utilization of LSTM neural network for water production forecasting of a stepped solar still with a corrugated absorber plate*. Pages 273-282.

This study introduces a long short-term memory (LSTM) neural network model to forecast the freshwater yield of a stepped solar still and a conventional one. The stepped solar still was equiped by a copper corrugated absorber plate. The thermal performance of the stepped solar still is compared with that of conventional single slope solar still. The heat transfer coefficients of convection, evaporation, and radiation process have been evaluated. The exergy and energy efficiencies of both solar stills have been also evaluated. The yield of the stepped solar still is enhanced by about 128 % compared with that of conventional solar still. Then, the proposed LSTM neural network method is

utilized to forecast the hourly yield of the investigated solar stills. Field experimental data was used to train and test the developed model. The freshwater yield was used in a time series form to train the proposed model. The forecasting accuracy of the proposed model was compared with those obtained by conventional autoregressive integrated moving average (ARIMA) and was evaluated using different statistical assessment measures. The coefficient of determination of the forecasted results has a high value of 0.97 and 0.99 for the conventional and the stepped solar still, respectively.

- **Keywords:** Stepped solar still; Corrugated absorber plate; Forecasting; LSTM neural network

Behzad Nazari, Mohammad Hossein Keshavarz, Majid Hosseinzadeh Mobarhan. *The simplest method for reliable prediction of autoignition temperature of organic hydroxyl compounds to assess their process safety in industrial applications*. Pages 283-290.

The knowledge of autoignition temperature (AIT) is essential for the manufacture, processing, handling, transport, and storage of combustible materials but its measurement is very laborious. This work introduces a simple model for estimating AIT of different classes of organic hydroxyl compounds containing the other polar groups such as –O–, –S–, –CN, –C(=O)O–, –NH2 and > NH. The new correlation can predict the AIT of any organic compounds including the hydroxyl functional group through its molecular structure. It is based on the number of hydrogen atoms and two correcting functions under certain conditions. Various types of statistical parameters including internal and external validations are done to assess the reliability of the new model. The high reliability of the new model is compared with the outputs of two of the best available predictive methods. It is indicated that the values of Mean Absolute Percent Error (MAPE) of the new model for both training and test sets, corresponding to 109 organic hydroxyl compounds, is 3.90 K, which is much less than two comparative methods, i.e. 7.81 and 13.70 K.

- **Keywords:** Autoignition temperature; Organic hydroxyl compound; Correlation; Molecular structure; Safety

F. Mohammadi, Sh. Mokhtari, A. Naderifar. *Statistical optimization of electrochemical conversion of heavy fuel oil to valuable products using response surface methodology*. Pages 291-301.

Mediated electro-membrane oxidation was employed to convert a refinery heavy fuel oil (HFO) to valuable liquid and solid products (heavy residuals) at mild conditions. Response surface methodology (RSM) was engaged to obtain maximum conversion of HFO by implementing the central composite design (CCD). Based on the prediction and optimization functions, the optimum conditions for HFO conversion were then established. When Ag (I) concentration, HFO content, electrolysis temperature and time were adjusted to 0.56 M, 1.2 wt. %, 32 °C and 11 min, respectively, the HFO converted to a liquid product comprising 10 % gasoline and kerosene, 20 % atmospheric gasoil, 40 % vacuum gasoil and 30 % vacuum residuals. These were very close to the model predictions representing reliability of the RSM technique. FTIR results after electrochemical conversion confirmed the production of branched aliphatic groups and regeneration of interacting hydroxyl and carbonyl groups for heavy residuals and liquid products. Sim-Dist results revealed that during the indirect electrolysis, cracking of the initial HFO to lighter products occurred. Besides, surface morphology of the heavy residuals showed formation of a calcined coke. Some pores and agglomerated asphaltenes were observed which are likely linked to the former presence of resinous components removed by electrolysis.

- **Keywords:** Heavy fuel oil; Mediated electro-membrane oxidation; RSM; Ag (II)

Saleh Abo-Elfadl, Mohamed S. Yousef, Hamdy Hassan. *Energy, exergy, economic and environmental assessment of using different passive condenser designs of solar distiller*. Pages 302-312.

An assessment of using different passive condenser designs of the solar distiller based on productivity, exergy, energy, energyeconomic, exergyeconomic, enviroeconomic is investigated experimentally. Five different condenser designs are considered; (i) glass plate condenser, GC (CSS), (ii) corrugated aluminum sheet heat sink condenser, CHS, (iii) aluminum heat sink condenser having vertical rectangular fins at its outer surfaces, RHS, (iv) aluminum heat sink condenser having pin fins at its outer surface, PHS, and (v) aluminum heat sink condenser having pin fins at its outer and inner surfaces, DPHS. The findings show that augmenting the rate of condensation by varying the condenser design increases the still yield to a limit and then decreases this yield at a higher condensation rate. CSS has the smallest freshwater yield and still with PHS has the maximum production with an increment of 54 % comparing with GC condenser. The maximum increase of the daily average energy and exergy efficiencies of the still is about 55.3 % and 73.1 %, respectively in case of PHS condenser compared with CSS. Still with DPHS condenser has the maximum production cost while the still with PHS or CHS condenser has the minimum. Distiller with PHS condenser is the best system in achieving CO2 reduction benefits of 1.82 tons CO2/year.

- **Keywords:** Solar still; Condenser design; Energy; Exergy; 4E analysis; Assessment

Morteza Jalali Alenjareghi, Alimorad Rashidi, Abbass Kazemi, Ahmad Talebi. *Highly efficient and recyclable spongy nanoporous graphene for remediation of organic pollutants*. Pages 313-322.

Spongy carbon nanostructures are prepared by using nanoporous graphene (NPG), single-wall carbon nanotubes (SWCNTs) and multi-wall carbon nanotubes (MWCNTs). For absorbing oil spills from the surface of water the sponges were made. The characterization of the sponges and their related substratum materials are performed by XRD, BET, FT-IR, TGA and DTA; the results were then evaluated by SEM and TEM; and the adsorption capacities were measured. Having changed the powder form to sponge, a 5.01 (g. g−1) enhancement of adsorption was seen for SWCNT and there was also a 14.07 (g. g−1) increase in MWCNT. The 176.33 (g. g−1) adsorption capacity of the nanoporous graphene sponge towards chloroform was a big surprise which was partly related to the powder's own high adsorption, 155.46 (g. g−1). In other word, an increase of 11–14% was observed in adsorption capacity of nanoporous graphene in sponge in comparison to powdery form. In addition, nanoporous graphene sponge (NPGS) is demonstrated to be perfectly recyclable and versatile, having been recycled through heat treatment, solvent extraction and mild-suction filtration with proper recovery ratios. The obtained recovery capacities of the three methods were 99.01, 98.50, and 98.05 %, respectively. Surprisingly, the adsorption capacity of the NPGS reached up to 98 % even after it was used 10 times. Based on a proper performance of NPGS, it can be a great candidate for oil spill cleanup.

- **Keywords:** Spongy nanoporous graphene; Remediation; Organic pollutant; Oil uptake capacity

Masaki Takaoka, Yingchao Cheng, Kazuyuki Oshita, Tomoaki Watanabe, Shoji Eguchi. *Mercury removal from the flue gases of crematoria via pre-injection of lime and activated carbon into a fabric filter*. Pages 323-332.

The emissions from crematoria have been identified as a source of mercury not currently being remediated. However, the effects of changing the operational conditions by

installing a fabric filter (FF) to remove mercury from the flue gas of a crematorium have not been examined in detail. In this study, the mercury concentrations of crematoria flue gases before and after passing through a pre-treated FF and a selective catalytic reactor (SCR) were recorded via continuous emission monitors to examine the effect of pre-injecting a mixture of lime and 10 % activated carbon into the flue. After the filter was installed and treated, mercury concentrations at the outlet of the SCR were very low, with a maximum of less than 5 μg/Nm3. The mercury removal efficiency ranged from 87.5–99.9%. The thick layer of lime and activated carbon on the surface of the FF effectively suppressed the peak mercury concentration at the outlet of the SCR. The relationship between the average mercury concentration at the inlet of the FF and the age of the person at death indicates that the age at death could be a key factor in controlling mercury emissions from a crematorium.

- **Keywords:** Mercury; Crematorium; Pre-injection; Fabric filter; Activated carbon

Guojin Qin, Changqing Gong, Yihuan Wang. *A probabilistic-based model for predicting pipeline third-party hitting rate*. Pages 333-341.

Third-party damage (TPD) is a severe threat to the integrity of the in-service oil and gas pipeline. This work aims to develop a probabilistic model to predict the hitting rate of pipelines by third-party excavation under a dynamic, uncertain process, which is subjected to the impact of the effectiveness of various preventative practices. In this work, a Bayesian network (BN) was utilized to predict the hitting rate on the pipeline by third-party excavations, in conjunction with the Markov process. The effectiveness of typical industry prevention practices (e.g., one call system) against third party damage was considered. The uncertainty associated with survey samples for the qualitative assessment of the effectiveness of prevention practices was addressed using the bootstrap technique. The presented methodology can provide a complete probabilistic description of the uncertainty associated with pipeline hitting.

- **Keywords:** Pipeline; Third-party damage; Bayesian network; Markov process; Bootstrap technique

Masoud Barani, Saeed Bazgir, Mahsa Keyvan Hosseini, Parisa Keyvan Hosseini. *Eco-facile application of electrospun nanofibers to the oil-water emulsion separation via coalescing filtration in pilot- scale and beyond*. Pages 342-357.

In the present environmental study, different polymer nanofibers as coalescing filters and the effect of their type on the separation of secondary oil emulsion from oily wastewater were investigated in a semi-industrial scale. Polystyrene (PS), polyacrylonitrile (PAN), and polyamid6 (PA6) were used to be electrospun on the polyester (PET) nonwoven substrates. These nanofibers were fabricated in various spinning times. Filtration variables were examined and a system was designed. By adding the nanofiber layer to the nonwoven substrate, pressure drop and coalescing filter efficiency increased in all samples. The separation efficiency for three nanofibrous coalescing filters in 20 min electrospinning of different polymers at the same condition on polyester nonwoven as substrate such as two nonwoven layers of PET and one layer of PAN, two nonwoven layers of PET, and one layer of PA6, two nonwoven layers of PET and one layer of PS were 89.3 %, 83.3 % and 69.8 % respectively. This value was 60.6 % for the blank sample (nonwoven polyester). Hence, the mixture of two nonwoven layers of PET and one layer of PAN was selected as the suitable filter. Using the suitable coalescing filter COD decreased significantly. It diminished the potential risks related to oil discharge to the environment.

- **Keywords:** Oil-water separation; Coalescing filtration; Nanofiber; Emulsion; Environment

Sandip Roy, Rohit Kshirsagar. *Development of risk acceptance criteria in the Indian context*. Pages 358-369.

There is a vital need for India to adopt risk acceptance criteria (RAC) relating to major hazard industries as it attempts to transform into a major global economy over the coming decades. The present work develops a generalized methodology for establishing RAC, and demonstrates its application in the Indian context. Risk levels from a wide range of natural and technological hazards faced by Indian people is analysed vis-à-vis those of select developed and other emerging economies. It is argued that despite the divergence of key risk metrics and socio-economic parameters – per capita GDP, average wage, value of statistical life, and the degree of risk aversion – between India and representative developed economies, it is viable to align the prospective RACs for India with best global guidelines. Based on the ALARP principle, for employees and the public, the intolerable individual risk levels are projected to be 10−3 and 10-4/year respectively, while the broadly acceptable level for both is proposed to be 10-6/year. For the societal RAC, the slope of the benchmark F–N curve is fixed at -1.0, while for a maximum of 10 human fatalities the anchor intolerable and acceptable frequency points are suggested to be 10−3/year and 10-5/year, respectively. It is hoped that these benchmarks would help regulatory intensification, and a strategic mitigation of both technological and natural hazards encountered in India.

- **Keywords:** Individual risk; Societal risk; Risk acceptance criteria; ALARP; Emerging economy

Zhijian Zheng, Zhong Chen, Zhibin Zhang, Guoxuan Xiong, Jiahua Zhu, Zhuyao Li. *Simultaneous PM2.5 and moisture removal from wet flue gas by a gas-liquid cross flow array*. Pages 382-391.

A gas-liquid cross-flow array (GLCA) system is proposed as the direct condensing technique for PM2.5 and moisture simultaneous removal from the wet flue gas. Such a GLCA with huge surface area is formed by numerous vertically down-flowing wastewater films along a number of wires through a perforated distributor. And each falling film acts as an independent sink to remove PM2.5 and moisture. Analytical models are developed to predict PM2.5 and moisture removal efficiency of a GLCA, based on the differential equation of convection diffusion with diffusiophoresis (DP), the only considering mechanism of PM2.5 removal. The models indicate that PM2.5 removal efficiency is proportional to the moisture removal amount, and PM2.5 removal efficiency can be increased sharply due to moisture condensation. Experiments with a lab-scale GLCA are carried out with variable humidity of inlet gas, and a constant gas (60℃) and water (20℃) temperature. The experimental measurements for PM2.5 and moisture removal generally compare satisfactorily with the model predictions.

- **Keywords:** PM2.5; Moisture removal; Condenser; Exhaust gas; Diffusiophoresis; Gas liquid cross flow

Krishnasamy Sivagami, Perumal Tamizhdurai, Shaikh Mujahed, Indumathi Nambi. *Process optimization for the recovery of oil from tank bottom sludge using microwave pyrolysis*. Pages 392-399.

Petroleum refining generates hazardous sludge with polyaromatic hydrocarbons and heavy metals. The main objective of the study was to evaluate the performance of microwave pyrolysis for the recovery of oil from furnace oil sludge. The characteristics of furnace oil tank bottom sludge such as pH, moisture, viscosity, and volatile hydrocarbon content were determined. Thermal Gravimetric Analysis has been done to determine the cracking and degradation range of oily sludge. Gas Chromatography-Mass Spectrometry was used to fingerprint the hydrocarbon. Pyrolysis experiments were conducted in lab-

scale pyrolysis set up with different susceptors and sludge in a specific weight ratio. The process parameters like microwave power, sludge: susceptor ratio were optimized to increase the oil yield. Graphite mixed sludge in 1:5 ratio at 450 W power shown higher oil yield. The calorific value of oil and char were determined as 44,442.9 and 16,686.58 kJ /kg. Physicochemical characteristics of oil such as flash point, density, and kinematic viscosity are 94 °C, 874.9, kg/m3, and 4.063 cSt. Cetane index and sulfur content were measured as 40.9, 6.85 g/kg respectively. The gas analysis had shown the presence of H2, CO2, CO, and CH4 compounds. Char contains a higher percentage of carbon, Fe, Al, Ni, Pb, Cd, and S compounds.

- **Keywords:** Tank bottom sludge; Microwave process; Pyrolysis; Susceptor; Recovery; Furnace oil

Wan Jiang, Xiangyu Xu, Zhihui Wen, Le Wei. *Applying the similarity theory to model dust dispersion during coal-mine tunneling*. Pages 415-427.

With the improvement of coal mine driving mechanization, the mining efficiency has been greatly improved. However, the problem of coal dust pollution becomes more serious. In order to improve the environment and dust removal efficiency of tunneling face, it is necessary to master the law of dust migration under the condition of dynamic coal cutting in fully mechanized tunneling face. Therefore, based on the similarity theory and the theory of gas-solid two-phase flow, the numerical simulation and similarity experiments are used to study the distribution of dust concentration and the dust diffusion characteristics in fully mechanized tunneling face with variable dust sources under the condition of forced ventilation. The results show that because of the difference of air velocity in the attachment area of impinging jet, the initial velocity and direction of the dust released from different dust sources are obviously different. The dust from the upper sources moves upward under the influence of the initial airflow, which causes high concentration of the roadway. While the dust from the lower sources moves downwards with the airflow, which hinders the dust flying to a certain extent. The dust diffusion range and concentration are significantly reduced in the case of lower dust source, and most of the dust moves along the bottom of the roadway or stays on the roadway floor. In addition, the similar experimental results of air velocity and dust concentration correspond well to the simulation results, which verifies the reliability of the simulation. These results are expected to provide a basis for the reasonable arrangement of dust prevention measures in fully mechanized tunneling face and improve the working face environment more effectively.

- **Keywords:** Fully mechanized tunneling face; Dust source location; Flow field structure; Dust migration

Carmen M. Sánchez-Arévalo, Álvaro Jimeno-Jiménez, Carlos Carbonell-Alcaina, María Cinta Vincent-Vela, Silvia Álvarez-Blanco. *Effect of the operating conditions on a nanofiltration process to separate low-molecular-weight phenolic compounds from the sugars present in olive mill wastewaters*. Pages 428-436.

The efficiency of nanofiltration to purify the tyrosol present in the olive mill wastewaters (OMWWs) has been studied. The similar molecular weight of tyrosol and the sucrose existing in this kind of by-products restricts the discrimination between both molecules through a membrane process, but the interest of phenolic compounds to be applied in cosmetics and pharmacology greatly motivates its recovery at the highest purity possible. Thus, two different simulated OMWWs composed of tyrosol and mixtures of tyrosol and sucrose, respectively, were nanofiltered using the NF270 membrane. Three transmembrane pressures (TMPs) and three cross-flow velocities were tested. The

optimum results were obtained at 0.5 m·s−1 and 15 bar. The rejections of the chemical oxygen demand (COD) were above 78 %, whereas phenolic compounds were barely retained. This indicates that the sugar was accurately separated from tyrosol, which was recovered in the permeate stream at a high purity.

- **Keywords:** Nanolfiltration; Olive mill wastewater; Phenolic compounds; Sucrose; Separation

Vahid Aryai, Rouzbeh Abbassi, Nagi Abdussamie, Fatemeh Salehi, Vikram Garaniya, Mohsen Asadnia, Al-Amin Baksh, Irene Penesis, Hassan Karampour, Scott Draper, Allan Magee, Ang Kok Keng, Chris Shearer, Suba Sivandran, Lim Kian Yew, Denham Cook, Mark Underwood, Andrew Martini, Kevin Heasman, Jonathan Abrahams, Chien-Ming Wang. *Reliability of multi-purpose offshore-facilities: Present status and future direction in Australia*. Pages 437-461.

Sustainable use of the ocean for food and energy production is an emerging area of research in different countries around the world. This goal is pursued by the Australian aquaculture, offshore engineering and renewable energy industries, research organisations and the government through the "Blue Economy Cooperative Research Centre". To address the challenges of offshore food and energy production, leveraging the benefits of co-location, vertical integration, infrastructure and shared services, will be enabled through the development of novel Multi-Purpose Offshore-Platforms (MPOP). The structural integrity of the designed systems when being deployed in the harsh offshore environment is one of the main challenges in developing the MPOPs. Employing structural reliability analysis methods for assessing the structural safety of the novel aquaculture-MPOPs comes with different limitations. This review aims at shedding light on these limitations and discusses the current status and future directions for structural reliability analysis of a novel aquaculture-MPOP considering Australia's unique environment. To achieve this aim, challenges which exist at different stages of reliability assessment, from data collection and uncertainty quantification to load and structural modelling and reliability analysis implementation, are discussed. Furthermore, several solutions to these challenges are proposed based on the existing knowledge in other sectors, and particularly from the offshore oil and gas industry. Based on the identified gaps in the review process, potential areas for future research are introduced to enable a safer and more reliable operation of the MPOPs.

- **Keywords:** Blue economy; Ocean multi-use; Offshore platforms; Structural integrity; Reliability analysis

Zhaoyuan Ma, Dong Yao, Jiangang Zhao, Huiyuan Li, Zhengrun Chen, Peizhe Cui, Zhaoyou Zhu, Lei Wang, Yinglong Wang, Yixin Ma, Jun Gao. *Efficient recovery of benzene and n-propanol from wastewater via vapor recompression assisted extractive distillation based on techno-economic and environmental analysis*. Pages 462-472.

N-propanol and benzene are important chemical organic compounds, which widely exist in wastewater of chemical industry, medicine and other fields. Because they form azeotrope with water, extractive distillation was used to separate them. In order to increase the efficiency of energy utilization, vapor recompression technology was added on the basis of extractive distillation. On the basis of vapor recompression assisted extractive distillation, energy integration was carried out according to pinch technology, and the optimal energy utilization method was found. The exergy loss and gas emission of each process were studied and analyzed. The results show that the vapor recompression assisted distillation process with feed preheating can reduce the heat duty and gas emissions, and improve exergy efficiency and economic performance. Therefore,

the vapor recompression assisted distillation process with feed preheating can effectively treat the wastewater containing benzene / n-propanol. It has the advantages of low cost, energy saving and environmental protection, which is of great significance to the development of environmental protection industry.

- **Keywords:** Ternary azeotropic mixtures; Vapor recompression; Extraction distillation; Energy saving; Economic optimization

Himanshu Manchanda, Mahesh Kumar. *Thermo-techno-economical experimental evaluation of a stepped solar distillation system with energy loss utilization*. Pages 473-481.

The aim of the present experimental work is to develop a new approach to utilize the underneath space of stepped basin solar distillation unit for drying agro-commodities. Two major solar applications are integrated to utilize the undesired energy losses. A stepped basin solar distillation-cum-drying unit (SBSD-DU) integrated with a parabolic reflector is thermally and economically analyzed. The effects of flow rates on the performance of distillation and drying unit are also evaluated. The internal and external heat transfer coefficients for distillation unit were found in the range of 56.35–125.28 W/m2oC and 17.54–20.85 W/m2oC, respectively. The distillate output at lower flow rate (50 mL/min) has been observed nearly 15 % higher than at higher water flow rate (65 mL/min). Maximum condensate yield of 3 L/m2/day with maximum energy and availability efficiency of 22.75 % and 2.2 %, have been obtained. Around 80 % moisture on the wet basis has been observed to evaporate from the dried agro-commodities (ginger/bitter gourd/potato slices). The unit cost of the distilled water and dried commodity is calculated as $ 0.0245. The experimental uncertainty is evaluated in the range of 3.99–4.45 %.

- **Keywords:** Stepped basin; Solar distillation; Drying of agro-commodity; Cost analysis; Flow rate; Availability efficiency

Dominik Bałaga, Michał Siegmund, Marek Kalita, Ben J. Williamson, Andrzej Walentek, Marcin Małachowski. *Selection of operational parameters for a smart spraying system to control airborne PM10 and PM2.5 dusts in underground coal mines*. Pages 482-494.

Airborne dust in underground hard coal mines is an ongoing explosion and respiratory health hazard. The latest design solution for controlling dusts, the smart spraying system, is described. From the results of stand tests, the main factors determining the efficiency of the new device are: 1) the integrated real-time acquisition of dust particle size and concentration data, determined using a new optical dust meter; 2) the fractional distribution of water droplets; and 3) the selection of droplet size to capture PM10 and PM2.5. The latter two factors are automatically controlled, based on dust measurements, by varying the pressure of water and compressed air supplied to the sprayer nozzles. The effects of varying these parameters and the results of stand tests are presented. The spraying device was tested for the effectiveness of PM2.5 dust and PM10 dust reduction in underground conditions in the KWK Pniówek mine. The tests were based on the following Polish Standards: PN-91/Z-04030/05 and PN91/Z-04030/06, which define the methodology for measurements of inhalable and respirable dust at workplaces using the filtration-weighing method to determine the concentration of inhalable and respirable dust with the spraying system on and off. The results showed that the assumed objective, i.e. development of a dust control device that would reduce PM2.5 dust (by min. 25 %) and PM10 dust (by min. 20 %) more effectively than the currently used solutions, was achieved in the project. At the same time, the device, due to application of dust sensor, continuously adjusts the parameters of spraying streams to the dust concentration level, optimizing the consumption of water and compressed air. Similar

results in reduction of PM10 and PM2.5 dust, with an average effectiveness of over 60 % is the undoubted advantage of the device.

- **Keywords:** Coal dust; Particle diameter; Dust suppression; Water-air spraying device

Mohammed O.J. Azzam, Saja A. Hazaimeh. *Olive mill wastewater treatment and valorization by extraction/concentration of hydroxytyrosol and other natural phenols*. Pages 495-523.

Olive mill wastewater (OMW) is a by-product generated from olive oil extraction systems. It contains high concentrations of organic compounds mainly phenols which cause environmental problems for the ecosystem, such as soil contamination and water pollution. Therefore, treatment of OMW is very much needed. Some of the naturally present chemicals in OMW have a positive economic value. In this investigation, liquid/liquid extraction using ethyl acetate (EA) as a solvent to recover such valuable compounds was investigated. Several parameters were studied namely, time of extraction, pH, EA/OMW volumetric ratio, and initial concentration of total phenols. Based on UHPLC analysis, hydroxytyrosol (HT) was the most abundant phenol in EA extracts from OMW. Many other phenols (tyrosol, oleuropein, p-coumaric acid, syringic acid, and 4-hydroxybinzoic acid) were also identified. Percentage recovery of HT reached 62 % after 2 h of extraction, at an EA/OMW ratio of 2/1 (v/v) and a pH of 2. Distribution coefficient of HT in EA was evaluated and was found to be around 0.8. The above process is envisioned to ultimately produce clean water which may be used in irrigation or in olive mills in a sustainable way. In addition, the extract is expected to have a high economic value.

- **Keywords:** Distribution coefficient; Ethyl acetate; Hexane; Hydroxytyrosol; Phenols; Valorization

Xiaohang Zhang, Xuewei Zhang, Yanping Liu, Qing Zhang, Shipeng Yang, Xuwen He. *Removal of viscous and clogging suspended solids in the wastewater from acrylonitrile-butadiene-styrene resin production by a new dissolved air release device*. Pages 524-535.

The suspended solids in the acrylonitrile-butadiene-styrene(ABS) wastewater are in the form of viscous latex, which strengthens the blocking phenomenon of the release device, increases the suspended solids in the return water and reduces the removal effect of the air flotation apparatus. Therefore, we designed a new release device. To achieve the goal of controlling the bubbles in the target diameter and enlarge the hole size as much as possible to reduce blockage, we studied the relationship between the geometry structure and performance of the new, which could be describeed by fixed polynomials. The best demulsification effect could be obtained by the hybrid of the polyferric sulfate and FO4440SSH, and the highest removal rate was 92.51 %. After a long-running in the ABS sewage treatment plant of the petrochemical industry, the removal rate of the new could maintain at a high level(>90 %), and the removal effect was stable. Compared with other release devices that reported in the literatures, the new one had advantages significant in both removal efficiency and operation cost.

- **Keywords:** Acrylonitrile-butadiene-styrene wastewater; Dissolved air flotation; The volume of gas release; The flow rate of gas release; Demulsification

C. Bretas Alvim, S. Castelluccio, E. Ferrer-Polonio, M.A Bes-Piá, J.A. Mendoza-Roca, J. Fernández-Navarro, J.L. Alonso, I. Amorós. *Effect of polyethylene microplastics on activated sludge proces: accumulation in*

***the sludge and influence on the process and on biomass characteristics*. Pages 536-547.**

According to previous research, it has been proved that wastewater treatment plants (WWTPs) can retain more than 90 % of the MPs contained in wastewater. However, a significant fraction of the MPs removed in WWTPs is retained in the sludge floc and this may lead to an environmental issue since biosolids can be used as fertilizers. The purpose of this research was to evaluate how the presence of polyethylene (PE) could interfere with the activated sludge performance. For this, a sequencing batch reactor (SBR) was continuously fed during 93 days with synthetic sewage and PE microbeads. It was observed that 98 ± 2% of the total amount of MPs that entered SBR was accumulated in the activated sludge. Despite the high accumulation of MPs in the sludge, the depuration performance of the reactor was not compromised. However, the presence of MPs decreased the richness (Chao1) and abundance-based coverage estimators (ACE) and diversity (Shannon) of the bacterial community on day 93. Based on the analysis of the diversity indices and the relative abundances of microbial taxa, it was concluded that MPs had selective effects on activated sludge microbial community. However, MPs did not affect the abundance of nitrifying and denitrifying bacteria in the sludge.

- **Keywords:** Activated sludge; Polyethylene; Microplastic; SBR

Jacek Grabowski, Krzysztof Korczak, Aleksandra Tokarz. *Aquatic risk assessment based on the results of research on mine waters as a part of a pilot underground coal gasification process*. Pages 548-558.

One of the possible applications of available hard coal resources is their underground gasification directly in the deposit. The gas obtained in this way is discharged to the surface for use in chemical synthesis or energy purposes. The environmental risk of the technology is mainly related to the potential negative impact of the process on groundwater and surface water, due to the need to remove process condensates and the drainage of the exploitation area. The risk occurs both during the process and after its completion. This article presents the results of a pilot study carried out in the Wieczorek Mine. The coal gasification experiment was carried out over 6 months (with 2 months of gas extraction) in real conditions in a georeactor located 450 m below the surface and on the surface of the object (cooling and cleaning system for gasification products). Water monitoring was carried out before the experiment, during the experiment and 5 years after the end of the process. The analysis includes the results of underground and surface water monitoring within the range of the potential impact of the pilot plant. The paper also presents the analysis of water-tar condensate collected from the gas cleaning system.

- **Keywords:** Wastewater; Underground coal gasification; Georeactor; Groundwater pollution; Monitoring

Jo Yee Ho, Denny K.S. Ng, Yoke Kin Wan, Viknesh Andiappan. *Synthesis of wastewater treatment plant based on minimal waste generation cost: A material flow cost accounting (MFCA) approach*. Pages 559-578.

Wastewater treatment (WWT) is a mandatory process to ensure wastewater quality meets legislation requirements and to reduce environmental impacts. Many established WWT technologies are available in the market and the selection of such technologies is usually based on heuristics. However, technologies selected using heuristics may not be able to guarantee optimal economic performance. In this respect, it is important for manufacturing companies to synthesise a WWT process with minimum investment cost while meeting legislation requirements. Most manufacturing companies face issues to achieve this goal. Among these issues, is the fact that part of the investment invested

into a WWT process will be lost to waste (sludge cake) generation. The generated waste (sludge cake) will require additional high waste disposal costs. Therefore, to reduce the loss of investment in a WWT process, the waste generation cost and waste disposal cost must be minimised. This can be addressed via Material Flow Cost Accounting (MFCA), a management tool that quantifies material flows across physical and monetary values in a production process. Previous works had adapted the concept of MFCA for prioritisation of waste streams for waste recovery and minimisation of investment cost in processes with revenue streams. Thus, the objective of this paper is to extend the use of MFCA as a preliminary decision-making tool in the selection of WWT technologies with minimum waste generation cost. To illustrate the developed approach, a case study on sago-based WWT process is solved in this work. Based on the results, the synthesised WWT process from the developed model is capable of recovering as much as 93.3 % of the total operating cost back into the manufacturing process while minimising the waste generation cost to 6.7 % of the operating investment cost.

- **Keywords:** Material flow cost accounting (MFCA); Hidden costs; Wastewater treatment; Waste generation cost; Process synthesis

F.A. Essa, A.S. Abdullah, Z.M. Omara. *Improving the performance of tubular solar still using rotating drum: experimental and theoretical investigation*. Pages 579-589.

In the current work, we introduced, experimentally and theoretically, a modified technique of reducing the water depth as much as possible inside the tubular solar still using a rotating drum. The existence of the rotating drum inside the tubular solar still provides the lowest amount of basin water and creates a thin water film, which is evaporated quickly. So, the effect of using closed ends drum and open ends drum on the performance of tubular distiller was investigated. Besides, using the rotating drum increased the evaporative and exposure surface areas inside the tubular solar still. Moreover, the effect of different rotating speeds (0.02, 0.05, 0.1, 0.2, 0.5, 1.0, 2.0, 3.0, and 4.0rpm) on the performance of tubular distiller was investigated. Furthermore, the system was studied with and without wick. The results revealed that the speed of 0.05 and 0.1rpm obtained superior performance of tubular drum distiller with and without wick, respectively. In addition, at 0.1rpm and without wick, the productivity of the tubular drum still was improved by 121 % and 136 % for the closed ends and open ends drums, respectively. While, at 0.05rpm and with wick, the productivity of the tubular drum still was enhanced by 140 % and 175 % for the closed ends and open ends drums, respectively. Furthermore, with wick, the thermal and exergy efficiencies of the tubular drum still were 56.4 % and 3.45 % for the closed ends drum and 61 and 3.6 % for the open ends drum, respectively.

- **Keywords:** Drum solar still; Tubular solar still; Drum speed; Desalination; Exergy

Shengqiang Yang, Buzhuang Zhou, Chaojie Wang. *Investigation on coal spontaneous combustion in the gob of Y type ventialtion caving face: A case study*. Pages 590-603.

Gas and coal spontaneous combustion (CSC) compound disasters have become a common mode of serious accidents in coal mines. This study is aimed at revealing the characteristics of such compound disasters in the gob of Y-type ventilation fully mechanized top coal caving face with a high-level drainage roadway (HLDR) (hereafter referred to as "Y+HLDR" working face) and providing a theoretical basis for disaster prevention and control. With the W1310 fully mechanized working face of Gaohe Coal Mine taken as the research background, the distribution law of gas concentration field in the gob of the "Y+HLDR" ventilation mode under different air supply conditions was numerically simulated with the aid of COMSOL, and the area of gas and CSC compound disaster in the gob was divided quantitatively. The results show that data obtained from

the field experiment coincide with the simulation results, which verifies the effectiveness of the simulation; Meanwhile, with the increase of air supply volume, the gas concentration near the working face is significantly reduced, and high-concentration gas is transferred to the deep part of the gob. The area where CSC induces gas explosions is divided by superimposing the gas and oxygen concentration fields that meet the conditions of compound disaster occurrence on the gob floor. It is concluded that the range of area with compound disaster risk is positively correlated with the air supply volume. The results of the simulation provide important theoretical guidance for the prevention and control of gob disasters.

- **Keywords:** Y-type ventilation; Coal spontaneous combustion; Gas explosion; Compound disaster; Similarity theory; Numerical simulation

V.R. Moreira, Y.A.R. Lebron, L.V.S. Santos, E. Coutinho de Paula, M.C.S. Amaral. *Arsenic contamination, effects and remediation techniques: A special look onto membrane separation processes*. Pages 604-623.

In many countries, arsenic (As) concentrations above acceptable standards for drinking water have been found, which is bringing awareness and becoming a worldwide concern. As occurs in the environment naturally, but anthropogenic activities such as mining, fossil fuels burning, pesticide and herbicide application have been playing a major role in the As occurrence in groundwater and drinking water. The two inorganic arsenic ions As(III) and As(V) are ubiquitous in natural waters and pose significant health risks to humans even at low concentrations, for example, lung cancer, cirrhosis and myocardial infarction. Therefore, there is an increasingly search for technologies that have high removal efficiency, simplicity, cost-effectiveness, feasibility and lower chemical requirements. In this regard, this paper reviews the occurrence, exposure pathways, effects and removal technologies such as oxidation, flocculation, coagulation, adsorption, ion exchange and particularly membrane separation processes (MSP), with attention to the disadvantages and limitations of these technologies. Furthermore, integrated approaches between MSP and others are discussed. Lastly, emergent technologies in MSP such as forward osmosis, membrane distillation and electrodialysis were discussed and their efficiency and performance towards As retention was presented.

- **Keywords:** Arsenic; Membrane separation processes; Arsenic contamination; Fate and removal

Hongqing Zhu, Yujia Huo, Wei Wang, Xin He, Shuhao Fang, Yilong Zhang. *Quantum chemical calculation of reaction characteristics of hydroxyl at different positions during coal spontaneous combustion*. Pages 624-635.

Hydroxyl groups are one of the key factors for the development of coal spontaneous combustion. Although the reaction mechanism has been studied by many scholars, the effects of their positions in the molecule on the reaction characteristics have not been considered. In this paper, Ph−CH2−CH3 was selected as the basic unit to construct small coal molecule models with one hydroxyl at different positions. The microscopic parameters of each model were calculated by density functional theory (DFT), and the elementary reaction pathways and thermodynamic parameters of hydroxyl groups were explored. It was found that the hydrogen of OH is the active site of nucleophilic reaction, the CαH bond of α-phenethyl alcohol and the OH bonds of the other molecules are most vulnerable to oxygen. All the models can generate H2O in the process of oxidation, other products of alcoholic hydroxyl groups are highly active oxygen-containing free radicals, while that of phenolic hydroxyl groups are quinones or ketones. The results of intrinsic reaction coordinate (IRC) indicated that hydrogen captured by oxygen is endothermic, while the ·OH free radical capturing hydrogen is exothermic. The activation energy of oxygen capturing hydrogen is 98–182 kJ/mol, which shows that the reaction can occur in the middle stage of coal spontaneous combustion (70–120 ℃), and the reaction rate

gradually accelerate with the increase of temperature. In the same conditions, the order of the oxidation reaction rates is 2-ethyl phenol > 3-ethyl phenol > 4-ethyl phenol > α-phenethyl alcohol > β-phenethyl alcohol, which is the same as the order of reaction activities but opposite to that of activation energies. The research is helpful to strengthen the judgment of coal spontaneous combustion risk and the development of flame retardant.

- **Keywords:** Coal spontaneous combustion; Hydroxyl groups; Computational quantum chemistry; Reaction mechanism; Thermodynamic parameters

Jia Lin, Ting Ren, Yuanping Cheng, Jan Nemcik. *Laboratory quantification of coal permeability reduction effect during carbon dioxide injection process*. Pages 638-649.

CO2 geo-sequestration in unminable coal seams is one promising method to mitigate greenhouse gas emissions and would be a means of cleaner production. At the same time, the injected CO2 can enhance coalbed methane recovery and offsets the economic cost for CO2 transportation and injection. However, this technology is still at its primary stage and so far, no large scale of field CO2 injection has been implemented. One of the main difficulties encountered in this process is the permeability reduction induced by CO2 injection and as a result, the injection rate is sharply dropped in the later period. In this paper, detailed laboratory experiments are conducted to investigate the permeability reduction effects during CO2 injections. The dynamic permeability reduction effects are measured with the continuous CO2 injection under different confining pressure conditions. Permeability reduction effects of 13 %–77 % are obtained with respect to the CO2 exposure time in different testings. In low permeability scenario, the permeability reduction effects are severer. Specifically, when the absolute permeability is 1mD, 0.42mD, 0.18mD and 0.03mD, the permeability reduction is 13 %, 36 %, 48 % and 77 %, respectively. Compared with the coal triaxial adsorption tests, it is suggested that the permeability equilibrium is not equal to the adsorption equilibrium. The triaxial adsorption equilibrium process takes much longer time than that of permeability equilibrium process. Based on the testing results, a novel dynamic permeability model is proposed to illustrate the permeability evolutions. The existence of weak internal surface influences the matrix strain and the permeability. This model is also validated by other's experimental results and can be used for explaining coal seam permeability reduction effects of CO2 injection in coal seams.

- **Keywords:** Permeability reduction; CO2-ECBM; Geo-sequestration; Adsorption; Coal matrix swelling; Fracture

A. Toporov, O. Aleksieieva, P. Tretiakov. *Probabilistic approach of reliability evaluation for the tubular elements of the chemical equipment according to technical state changing*. Pages 650-663.

During the operation of chemical equipment, its technical condition, operating modes and operability change. Such phenomena are typical for the main element of chemical equipment - tubular elements, which must have the required strength, ensure the transportation of the working medium and the transfer of heat between the working medium. During the operation of tubular elements the wall thickness decreases, deposits appear on them, the wall roughness and the flow area change. The parameters that affect the change in the technical state are probabilistic in nature and can vary over a wide range. As a result, the operability of both tubular elements and the equipment in which they are installed decreases. To evaluate the performance of tubular elements under conditions of changes in their technical state, it is proposed to use three functioning criteria: strength, temperature and hydraulic. The strength criterion has the following meaning: the internal working pressure must not exceed the tolerance one; temperature criterion – the temperature of the working medium inside the tubular

element must be within the specified range; hydraulic criterion – the pressure drop must not exceed the tolerance value. It has been developed a probabilistic mathematical model that allows one to determine the criterion parameters under the assumption that the influencing factors have a normal distribution law and are described by their mathematical expectation and standard deviation. The proposed method allows, with a given level of reliability, to substantiate the design parameters of tubular elements during their design taking into account changes in the technical state during operation.

- **Keywords:** Reliability evaluation; Technical state; Probabilistic analysis; Tubular element; Surface deposits

Jilai Cao, Jian Zhang, Xinhai Yu, Shan-Tung Tu. *Detection of pressure relief valve leakage by tuning generated sound characteristics*. Pages 664-675.

Currently, accurate on-line leakage detection of pressure relief valves (PRVs) is still a challenge. This study presents an innovative method of detecting PRV leakage by generating sounds with a crest at a frequency of 32.7 kHz and a trough at a frequency of 25.0 kHz using specially designed cavity-shaped whistles. The accuracy of the leakage detection using the proposed method was superior to that of the commercial acoustic emission method. On the one hand, this is because the interference by the leakage jet noise could be alleviated by the discernable sound spectrum generated using cavity-shaped whistles. On the other hand, this is because the occurrence of the crest (32.7 kHz) and trough (25.0 kHz) of the generated sounds was independent of the leakage flow rate, leakage channel size, and sensor location. The integration of the cavity-shaped whistle with the PRV showed negligible effects on the PRV dynamic performance. The proposed method showed great potential for the leakage detection of the PRV given its advantages of low cost, high sensitivity and good accuracy.

- **Keywords:** Leakage detection; Pressure relief valve; Sound characteristic; Cavity-shapedd whistle; Dynamic performance

Brian Gidudu, Evans M. Nkhalambayausi Chirwa. *Production of a bacterial biosurfactant in an electrochemical environment as a prelude for in situ biosurfactant enhanced bio-electrokinetic remediation*. Pages 676-685.

The possibility of producing biosurfactants in an electrochemical environment was studied at three different currents of 0.5 A, 1 A and 1.5 A. The Pseudomonas aeruginosa strain was able to produce a biosurfactant in all the three experiments with a yield of 36.25 ± 3.75 mg/mL, 22.5 ± 5 mg/mL, 6.25 ± 1.25 for 0.5 A, 1 A and 1.5 A respectively. A rhamnolipid biosurfactant with 7 mono-rhamnolipid and 4 di-rhamnolipid homologues was detected in all experiments. However, the survival and yield of the biosurfactant was affected by the intensity of the electric field applied. The highest electric field of 1.5 A led to the total inactivation and elimination of the bacteria within the first 12 h while the bacteria survived to the end of the experiment in 96 h when 0.5 A and 1 A was applied.

- **Keywords:** Rhamnolipid; Electrokinetic; Biosurfactant; In situ

Kongxing Huang, Guohua Chen, Faisal Khan, Yunfeng Yang. *Dynamic analysis for fire-induced domino effects in chemical process industries*. Pages 686-697.

Domino effects are typically high-impact low-probability (HILP) accidents, which pose a serious threat to chemical process industries. Previous researches on domino effects in chemical industries focus more on static analysis at the spatial scale. From the

perspective of the spatial and temporal characteristics of the accident, this study proposed a model to analyze dynamic evolution process of domino effects by using matrix calculation coupled with Monte Carlo simulation, and the dynamic propagation of pool fire accidents is considered as the evolution of domino effects. The algorithm of the model for dynamic domino probabilities considering the synergistic effects of multiple escalation vectors from different units can be used to analyze the complex scenarios of domino effects with high-level and multiple primary accident units. Moreover, the model can be applied in chemical areas with a large number of installations due to the greatly improved calculation efficiency. The proposed model is tested and validated using earlier studied dynamic Bayesian network method, and the application of the model is demonstrated on a complex multi-unit system. The results show that domino effects have strong temporal correlation, and the scenario with multiple primary accident units is much more serious than that with only one primary accident unit, which provide important support for the implementation of emergency response. The study highlights that the proposed model serves as an important tool to evaluate strategies for prevention and control of domino effects.

- **Keywords:** Domino effect; Dynamic probability; Chemical process industry; Monte Carlo

Bo Sun, Yu Li, Zili Wang, Dezhen Yang, Yi Ren, Qiang Feng. *A combined physics of failure and Bayesian network reliability analysis method for complex electronic systems*. Pages 698-710.

Complex electronic systems have a structures that can lead to coupling failure mechanisms and difficulties in collecting measured data. These issues increase the difficulty of reliability analysis. Current reliability research methods cannot effectively solve the above problems. In this paper, we propose a new approach that combines a physics of failure (PoF) method and a copula Bayesian network to assess complex electronic systems. The proposed approach improves the defects of PoF methods and traditional Bayesian networks when applied to the reliability analysis of complex electronic systems. A copula Bayesian network is used to realize the dependent failure modeling of modules or components for interlevel failure and intra-level failure. The PoF method addresses the difficulty in obtaining measured data. This proposed approach is applied to the reliability analysis of the integrated processor system in communication equipment. The key impacted subsystems and devices are analyzed from three aspects—qualitative analysis, forward inference and backward inference—and the corresponding failure life distributions are calculated. This method can guide the improvement of system reliability and system maintenance.

- **Keywords:** Reliability analysis; Bayesian network; Electronic system; Copula; Physics of failure

Peng Liu, Jinyang Fan, Deyi Jiang, Jiajun Li. *Evaluation of underground coal gas drainage performance: Mine site measurements and parametric sensitivity analysis*. Pages 711-723.

Underground gas extraction from coal formations has triple-effects involving mining safety, low-carbon gas capture and greenhouse gas control. Air leakage around the drainage borehole is a serious problem that continuously affects gas drainage performance. In this study, mine site measurement of gas drainage data is firstly performed in coal mine, and then a mechanism-based model is proposed to theoretically describe gas desorption and diffusion and flow through coal around the drainage borehole. Further, the propose model is numerically solved and verified with borehole drainage data measured in mine site. Followed this, the validated mechanism-based model is implemented to conduct parametric studies. The results showed that: (a) as the fracture permeability increases from 3 × 10−22 m2 to 3 × 10-14 m2, the air leakage

flux increases from 7355 m3/d to 18,303 m3/d, and the gas concentration decreases from 46.9 % to 12.7 %, it indicates that changing the permeability around the borehole may be a wise strategy to control air leakage; (b) the coal matrix parameters (including permeability, sorption constant and radius of matrix) have a dynamic impact on gas drainage performance at the different stage of gas drainage. For example, the increment of methane production induced by increasing the sorption constants does not exceed 3.3 % at the drainage time ~0.34 day; while the growth increases to more than 19.5 % at the drainage time ~ 9.75 days; (c) at the initial stage of extraction gas production is mainly determined by the fracture flow. A higher permeability of coal fracture will incur more air leakage flux, reducing gas concentration in drainage borehole; (d) whereas, the matrix parameters dominate gas flow at a later stage. Increasing matrix permeability, sorption property or decreasing the matrix radius will enhance the gas exchange flux from the pore system of coal matrix to the fracture system, subsequently incurring a higher concentration/production of drainage gas. The simulated result and field tests demonstrates that sealing on the coal wall around the borehole can block a portion of air leakage paths and reduce air leakage linearly, which illuminates a more efficient strategy to minimize air leakage for underground gas extraction.

- **Keywords:** Underground coal mine gas drainage; Air leakage; Numerical modeling; Fracture-matrix interaction

Chan Seok Jeong, Chi Young Lee. *Experimental investigation on spray characteristics of twin-fluid nozzle for water mist and its heptane pool fire extinguishing performance*. Pages 724-736.

Water mist, which is an alternative to halon fire-extinguishing agents, can maintain the clean environments and prevent the huge fire loss in diverse industrial fields. In the present experimental study, the spray characteristics of a twin-fluid nozzle for water mist and its heptane pool fire extinguishing performance were investigated. As the spray characteristics, the SMD (Sauter Mean Diameter) of water mist, discharged water flux distribution, downward air flow velocity, and inlet pressures of fluids were measured and analyzed. Subsequently, through the fire extinguishing experiments using three different heat release rate conditions, the fire extinguishing map, extinguishing time, water consumption, and water mist effect on the mass loss rate were examined in detail. In addition, the experimental data using the twin-fluid nozzle were compared and discussed with those using the single-fluid nozzle reported in a previous study. Based on the present experimental data of fire extinguishments, particularly under high air flow rate conditions, the twin-fluid nozzle showed high fire extinguishing performance. Moreover, compared with a previous study using the single-fluid nozzle, it was found that the twin-fluid nozzle can successfully extinguish liquid pool fire with shorter fire extinguishing times, lesser water consumption, and lower inlet pressures. Based on the present results, it was found that the air flow of the twin-fluid nozzle is an important factor that determines and affects its fire extinguishing performance. Further, the twin-fluid nozzle was found to possess a significant potential to considerably improve the performance of water mist fire suppression systems.

- **Keywords:** Twin-fluid nozzle; Water mist; Spray characteristics; Heptane pool fire; Fire extinguishing performance; Water mist fire suppression system

Kai Ye, Xiao Tang, Yuan Zheng, Xiaoyu Ju, Yang Peng, Hong Liu, Dong Wang, Bei Cao, Lizhong Yang. *Estimating the two-dimensional thermal environment generated by strong fire plumes in an urban utility tunnel*. Pages 737-750.

Although utility tunnels act as an innovative technique for the sustainable development of city's utilities and limited underground space today, the fire issues in this type of tunnel

should be carefully treated as they are different from traffic tunnel fire scenarios. In order to propose an easy-to-use two-dimensional (2D) temperature estimation methodology that is helpful to the designers, operators and firefighters, the temperature distributions and ceiling jet thickness (the vertical distance from the ceiling to where the temperature within the fire-induced smoke flow drops to half of its maximum at a certain location) were investigated with full-scale fire tests in a utility tunnel. The vertical temperature distributions were represented as a normalized single convex-concave profile. Self-similarity was confirmed and three types of similarity profiles were found. In order to correlate the inner boundary layer region and outer region of these ceiling jet flow profiles, a series of mathematical functions combining a power function and Gortler's error function were employed. Furthermore, the ceiling jet thickness was found to vary as a power function with the longitudinal distance, rather than being a constant as previous research suggested. The vertical distribution model, the ceiling jet thickness model and the longitudinal temperature decay model were combined into a framework to empirically estimate the 2D thermal environment generated by strong fire plumes in utility tunnel's fire protection engineering practice.

- **Keywords:** Utility tunnel; Fire safety; Ceiling jet; Vertical distribution; Two-dimensional temperature prediction

Marco Bellegoni, Federica Ovidi, Gabriele Landucci, Leonardo Tognotti, Chiara Galletti. *CFD analysis of the influence of a perimeter wall on the natural gas dispersion from an LNG pool*. Pages 751-764.

We developed an innovative tool to support the simulation of gas dispersion from liquefied natural gas pools in presence of obstacles. For the first time, the systematic evaluation of the influence of atmospheric stability conditions and the variation of the source term on congested dispersion scenarios is carried out, coupling integral models and computational fluid dynamics (CFD). The atmospheric boundary layer is implemented in the CFD together with ad-hoc boundary conditions, aimed at reproducing the dynamic pool spreading and consequent vaporization, simulated through integral models. A preliminary comparison is done between the results given by CFD and literature integral dispersion models in an open field case; subsequently, the presence of a perimeter wall is analyzed through the CFD technique. The results show a good agreement between the CFD and the integral models in the open field configuration, even though an overprediction of methane concentration is underlined for the integral model. In the case of the obstacle, CFD permits a precise analysis of the flow-field in all the considered atmospheric conditions and a deep investigation of the effects of the wall on the methane concentration.

- **Keywords:** CFD; Integral models; Liquefied natural gas; Consequence assessment; Gas dispersion; Protection wall

Youngjae Kim, Yosep Han, Sookyung Kim, Ho-Seok Jeon. *Green extraction of lithium from waste lithium aluminosilicate glass-ceramics using a water leaching process*. Pages 765-774.

An acid-free leaching process for lithium extraction from waste lithium aluminosilicate (LAS) glass-ceramics was investigated. Lithium was extracted by a water leaching process after calcination with CaO or a CaO-CaCl2 mixture. Compared to extraction using only CaO calcination, the addition of CaCl2 to CaO can significantly reduce the Si:Ca mixing ratio as well as the thermal treatment temperature. A drastic decrease in thermal treatment and leaching time was observed during the experiments. Based on thermodynamics calculations and X-ray diffraction analysis, the crystalline phase that determined the lithium extraction mechanism was investigated. In substituting CaO with CaCl2, the lithium leaching rate initially decreased or remained constant due to a decrease in the LiAlO2 phase. However, the lithium leaching rate gradually increased with

increasing CaCl2 substitution rate, caused by an increase in the formation of the LiCl phase. In addition to lithium, calcium and chloride were also observed during the water leaching process. The leaching rate was independent of the thermal treatment and leaching time. Considering conventional lithium purification techniques, a green process for lithium extraction, purification, and recovery from waste LAS glass-ceramics is proposed.

- **Keywords:** LAS glass-ceramics; Lithium; Calcination; Leaching; β-spodumene

Sajad Tamjidi, Bahareh Kamyab Moghadas, Hossein Esmaeili, Farideh Shakerian Khoo, Gholamhossein Gholami, Mansoure Ghasemi. *Improving the surface properties of adsorbents by surfactants and their role in the removal of toxic metals from wastewater: A review study*. Pages 775-795.

Heavy metals are pollutants that are naturally produced by human activities. Due to heavy metals' amount and toxicity in aqueous media, they are considered extremely harmful to human life. Therefore, it is necessary to find effective and efficient methods, as a severe challenge for reducing these pollutants to a permissible level. Among the various removal methods, the adsorption process has received much attention due to its benefits like low cost, ease of operation, high selectivity, and high removal efficiency. So far, various adsorbents such as activated carbon, agricultural waste, minerals, nanoparticles, and other inexpensive adsorbents have been used. Surface modification of these adsorbents by surfactants improves the adsorption properties, and as a result, enhances the adsorption capacity of adsorbents. This research has tried to discuss the use of surfactant-modified adsorbents to remove metal ions from aqueous media. In this study, heavy metals and various methods for removing them will also be studied. Also, isotherm, thermodynamic and kinetic behaviors of the sorption process are considered. The addition of anionic and cationic surfactants to the adsorbents can strongly alter the adsorbent's surface charge and directly affect the optimal pH value. Also, the maximum sorption efficiency using surfactant-modified adsorbents has been obtained at low temperatures (25 °C), which can be economically viable. According to previous studies, two surfactants such as SDS and CTAB, have shown a high ability to improve the adsorption efficiency and adsorption capacity of adsorbents. To this end, DNPH/SDS/Fe3O4 and CTAB/yeast adsorbents showed the highest removal efficiency (99.5%), which were able to remove Cr(VI) and CrO42− ions, respectively. Moreover, both adsorbents showed significant adsorption capacity.

- **Keywords:** Adsorption; Surfactants; Heavy metals; Wastewater treatment

Z.M. Omara, A.S. Abdullah, F.A. Essa, M.M. Younes. *Performance evaluation of a vertical rotating wick solar still*. Pages 796-804.

In this work, a new solar still desalination system named vertical rotating wick solar still (VRWSS) was investigated experimentally. The experiments were performed under different operating conditions. The performance of VRWSS was investigated under different wick belt materials (jute and cotton cloth), belt rotational speeds (0.02, 0.05, 0.1, 0.2, and 0.3 rpm), and rotating directions (clockwise and counterclockwise) with and without solar tracking. The VRWSS features are its small size (small horizontal area), fast water evaporation and condensation due to the low thermal capacity and large condensation area. The results revealed that the jute wick obtained higher productivity than the cotton wick at all belt rotational speeds except that at 0.02 rpm. Additionally, the water production for VRWSS-counterclockwise movement increased from 4350 mL/m2.day at 0.02 rpm to 5800 mL/m2.day at 0.05 rpm, then, the productivity started to decrease with increasing the speed. Furthermore, VRWSS productivity with counterclockwise movement was always larger than that with clockwise direction at all

rotational speed except at 0.02 rpm. Besides, the solar tracking for VRWSS (jute wick-counterclockwise-0.1 rpm) increased the freshwater productivity by about 37% with a thermal efficiency of 51%. The cost of produced freshwater from VRWSS was 0.02 $/L.

- **Keywords:** Wick solar still; Rotating wick; Rotating speed; Rotating direction; Solar tracking; Desalination

Manjun Yang, Hui Liu, Bo Ye, Wei Qian. *Recycling of printed circuit boards by abrasive waterjet cutting*. Pages 805-812.

The rapid growth of waste printed circuit boards (PCBs) necessitates development of compatible treatment techniques. In this study, abrasive waterjet (AWJ) cutting technology was utilized to crush waste PCBs for the first time. Cutting experiments were mainly performed on waste mobile mainboard, random access memory (RAM), universal circuit board (UCB), and central processing unit (CPU). The results demonstrated that AWJ cutting was capable of breaking waste UCB (~ 14 mm thick) into small particles (< 1 mm) in one-step processing, by which metals and nonmetals were well dissociated. SEM images of RAM and mainboard showed PCBs had a multi-layer structure, which would favor component dissociation under the mechanism of abrasive grinding. All the cutting debris of CPU (mainly Cu and Ti particles) were micro-sized (< 150 μm) and metals were completely dissociated. Mechanical property analysis showed tensile strengths of RAM, UCB, and CPU were 150.0, 72.3 and 74.4 Mpa, respectively, which were apparently lower than that of hard materials. This implied that AWJ cutting has a huge potential in enhancement of material-removal indicator through system improvement and process optimization. Thus, this study offers a promising environmental-friendly method for recovering metal resources from e-waste.

- **Keywords:** E-waste; Mechanical technology; Metal recovery; Abrasive waterjet

Parashuram Kallem, Israa Othman, Mariam Ouda, Shadi W. Hasan, Inas AlNashef, Fawzi Banat. *Polyethersulfone hybrid ultrafiltration membranes fabricated with polydopamine modified ZnFe2O4 nanocomposites: Applications in humic acid removal and oil/water emulsion separation*. Pages 813-824.

This study explored the impact of eco-friendly polydopamine (PDA) coated ZnFe2O4 nanocomposites (PDA@ZnFe2O4 NCs) as nanofillers to fabricate a new class of polyethersulfone (PES) hybrid ultrafiltration (UF) membranes for wastewater treatment applications. The hybrid UF membrane was prepared by incorporating PDA@ZnFe2O4 NCs into PES via the non-solvent induced phase separation (NIPS) process. The PDA@ZnFe2O4 NC was characterized by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Additionally, the morphology and performance of the prepared hybrid membranes were characterized by SEM, contact angle, surface charge, and thermogravimetric analysis (TGA). The incorporation of PDA@ZnFe2O4 NC into the PES membrane affects the porosity, mean pore radius, hydrophilicity, and thermal stability of the developed hybrid membranes. The pure water flux of the PES hybrid membrane with 4 wt% PDA@ZnFe2O4 reached ~687 L/m2 h, which is about 188% higher than that of the pristine PES membrane. The performance of the PES/ PDA@ZnFe2O4ultrafiltration hybrid membrane was also investigated using humic acid (HA) foulant and oil/water emulsion individually. Compared to the pristine PES and PES/ZnFe2O4 membranes, the developed hybrid membranes showed enhanced permeability and HA foulant removal. HA's removal efficiency has improved from ~65% in the pristine PES membrane to ~94% in the 4 wt% PDA@ZnFe2O4 hybrid membrane. The abundant functional groups on the PDA@ZnFe2O4 NC surface also enhanced the separation of the oil/water emulsion (96%). In both the HA and oil/water emulsion separation tests, the flux recovery ratio

(FRR) and reversible fouling ratio (Rr) were also significantly improved, suggesting that the PES/PDA@ZnFe2O4 membrane was a very promising candidate for HA removal and treatment of oily wastewater.

- **Keywords:** PDA coated ZnFe2O4nanocomposites; PES hybrid membranes; HA removal; oil/water emulsion separation; Anti-Fouling

J. José Torres, Macarena Cuello, N. Ariel Ochoa, Cecilia Pagliero. *Biodiesel wastewater treatment using nanofiltration membranes*. Pages 825-833.

Water reclamation and reuse are economically and environmentally important issues for industries. Costly and ineffective treatments such as coagulation, flocculation, and/or biological treatment are the most widely used technologies for these processes. The aim of this paper is to study membrane separation to treat biodiesel wastewater as an alternative. To achieve this goal, two commercial nanofiltration membranes were used to treat medium-high strength wastewater. An Inopor Nano tubular ceramic membrane was used in a cross-flow module and a NF99HF Alfa Laval polymeric flat sheet membrane was used in a dead-end filtration cell. Wastewaters were prepared and treated with these membranes achieving maximum fluxes of permeate of 53.1 L h-1 m-2 for the ceramic membrane and 12.2 L h-1 m-2 for the polymeric membrane at 20 bar and 30 °C. The results shows a chemical oxygen demand retention between 80–85 % were obtained for both membranes, while the retention of ionic species due to changes in electrical conductivity was 76–89 %. Transmembrane pressure, organic load, hydraulic permeability, cross-flow velocity, wastewater characterization and fouling resistance-in-series analysis were also made and analyzed in detail in order to explore the actual use of nanofiltration.

- **Keywords:** Membrane; Biodiesel wastewater; Dead-end; Cross-flow nanofiltration

Y.N. Chow, L.K. Lee, K.Y. Foo. *Scientific rationale of hospital discharge as a sustainable source of irrigation water: Detection, phytological assessment and toxicity verification*. Pages 834-845.

Hospital discharge (HD) represents the primary point source of pharmaceutical components that may constitute not only a sharp risk of phytotoxic effects in food crops, but leaving behind the toxicity implications to the environment. The present work has been oriented to the scientific assessment of pharmaceutical compounds in HD. The phenological, physiological, and morphological changes, oxidative stress biomarkers, antioxidative responses, bioaccumulation and bioconcentration factor in relation to different concentrations of HD-induced irrigation in Ipomoea aquatica were evaluated; while the cytotoxicity and genotoxicity on human hepatocellular carcinoma (HepG2) cell were assessed. Acetaminophen, metoprolol, atenolol, enalapril, and metformin were predominantly detected in the raw HD and bioaccumulated in I. aquatica. Concentration-dependent phenological inhibition, chlorophylls reductions, morphological distortions, reactive oxygen species generation, and antioxidant enzymes upregulation were recorded in the HD-irrigated I. aquatica. Drastic reductions in cell viability and increase of tail damage and tail moment indicated the metabolic alterations of mitochondrial function, and deoxyribonucleic acid (DNA) damage via oxidative stress and DNA adducts formation in the HD-treated groups. The diluted HD at 5% and 10 % could be feasibly reused for food crops irrigation, verified by the negligible phytotoxic implications in the plant model, bioaccumulation, and cytotoxic and genotoxic effects in HepG2 cell.

- **Keywords:** Cytotoxicity; Emerging organic pollutants; Genotoxicity; Hospital discharge; Phytotoxicity; Wastewater irrigation

Borja Ferrández-Gómez, Diego Cazorla-Amorós, Emilia Morallón. *Feasibility of electrochemical regeneration of activated carbon used in drinking water treatment plant. Reactor configuration design at a pilot scale*. Pages 846-857.

This work evaluates the feasibility of electrochemical regeneration of granular activated carbon used in drinking water treatment plants as a real alternative to thermal regeneration. Two pilot-plant-scale reactors, with a capacity of 10−15 kg, have been designed using two different configurations, parallel plate electrodes and concentric cylindrical electrodes. The optimization of the anode material has also been studied and Pt/Ti, RuO2/Ti and IrO2/Ti have been used. After the regeneration and, thus, recovery of the porosity the samples were tested in the adsorption of bisphenol A. In the electrochemical regeneration, recovery of the porosity of spent activated carbon until 100 % and 96 % with respect to the pristine activated carbon using Pt/Ti anode after 3 h of treatment, has been achieved. The regeneration process produces a small increase in the number of surface oxygen groups. No important differences have been observed among the tested anodes and RuO2/Ti and IrO2/Ti can be an economic alternative to Pt/Ti. Bisphenol A adsorption kinetics was slower in regenerated activated carbons probably due to the formation of surface oxygen groups. However, the adsorption capacity was similar in the regenerated samples and the pristine one.

- **Keywords:** Electrochemical regeneration; Activated carbon; Anode; Reactor configuration; Adsorption; Bisphenol A

Xiao Liu, Sen Yang, Shibo Liu, Yong Yang. *Performance and mechanism of phosphorus removal by slag ceramsite filler*. Pages 858-866.

Ceramsite made from BOF (basic oxygen furnace) slag was used in column test to deal with aquatic phosphate. The objective of this study was to identify the phosphorus (P) removal mechanisms of slag ceramsite and to evaluate its potential use in efficient phosphorus adsorption filter. The relationships of Ca2+, pH and phosphorus removal, as well as filler regeneration were investigated. Chemical extraction, SEM-EDX, XRD, FTIR, XPS were employed to determine the mechanisms of phosphorus removal. The slag-ceramsite column showed good adaptability for low strength phosphate. Results demonstrated that suitable HRT facilitated the efficient phosphorus removal for stable and long-term operating. As HRT was 2.8 h and influent PO4-P was 10 mg/L, the P-uptake capacity of ceramsite filler was 10.5 mg/g in 158 days. The P-uptake mechanisms of slag-ceramsite filler including surface adsorption, Ca2+/OH− release, and chemical precipitation. Weakly adsorptive phosphorus and precipitated calcium phosphate were dominant in the sequestered phosphorus. Amorphous Ca-deficient hydroxyapatite (CDHA) and carbonated hydroxyapatite (CO3-HA) were the dominant calcium phosphate phases. The exhausted ceramsite filler could be regenerated by NaHCO3 elution and calcination process.

- **Keywords:** Slag ceramsite filler; Phosphorus; Chemical extraction; CO3-HA; Regeneration

Junjie Kang, Yuguang Niu, Bo Hu, Hong Li, Zhenhua Zhou. *Dynamic modeling of SCR denitration systems in coal-fired power plants based on a bi-directional long short-term memory method.* Pages 867-878.

Selective catalytic reduction (SCR) denitrification system can effectively reduce NOx emission by controlling ammonia injection. However, the energy structures, load fluctuations, reactor dynamic characteristics and system delay pose great challenges to the precise ammonia injection. To achieve high-precision NOx emissions prediction, a method that combinations dynamic joint mutual information and Bi-LSTM is proposed,

where the dynamic joint mutual information theory is used to estimate the reactor dynamic characteristics and system delay. And then, the inputs of the Bi-LSTM are reconstructed according to the estimations. Thus, the Bi-LSTM is established to realize the accurate NOx estimation at the current time and t+3 moment of SCR outlet. Taking a 660MW tangent coal-fired boiler as an example, we establish the Bi-LSTM network by using more than 15,000 sampling data over 11 consecutive days, and predict NOx emissions. Experiments demonstrate that considering the dynamic joint mutual information and reconstructing the inputs, the Bi-LSTM network can greatly improve the prediction accuracy, which provides the basis for the realization of accurate ammonia injection and reduction of NOx emissions.

- **Keywords:** Bi-directional long short-term memory; Selective catalytic reduction system; Dynamic joint mutual information; Dynamic prediction model; NOx emission; Coal-fired utility boiler

Qunwei Wang, Jiexin Tang, Gyunghyun Choi. *A two-stage eco-efficiency evaluation of China's industrial sectors: A dynamic network data envelopment analysis (DNDEA) approach*. Pages 879-892.

Past studies used the network data envelopment analysis approach from a two-stage perspective (the production stage and waste/pollutant treatment stage) to evaluate industrial eco-efficiency and assess internal ineffective sources. However, these studies did not consider the dynamic features, i.e., capital investments in the current period are used to establish fixed assets for two stages, which can also be used in the later period, thus affecting its two-stage eco-efficiency. A dynamic network data envelopment analysis approach is adopted to fill this research gap and evaluate Chinese industrial two-stage eco-efficiency during 2010–2015, reflecting the practical production context and achieving comparable efficiencies among different periods. The major results of our study are: Firstly, not considering the dynamic features leads to an underestimation of the two-stage eco-efficiency. Secondly, the production efficiency was higher than the treatment efficiency, and the two-stage eco-efficiency was between the two during the study period. Furthermore, eastern China performed best with respect to the two-stage eco-efficiency, including production and treatment efficiencies, followed by the central and the western areas. Finally, a fifth of the 30 regions had a relatively low value of the input and output efficiencies of both production and treatment stages based on the clustering analysis.

- **Keywords:** Production stage; Pollution treatment; Production investment; Treatment investment; Slacks-based measure; Data envelopment analysis

Katsuhiro Okamoto, Toshikazu Ichikawa, Jumpei Fujimoto, Nobuyuki Kashiwagi, Masahiro Nakagawa, Takao Hagiwara, Masakatsu Honma. *Prediction of evaporative diffusion behavior and explosion damage in gasoline leakage accidents*. Pages 893-902.

To meet the requirements for use as an automotive fuel, motor gasoline must be highly flammable and combustible. In addition, because gasoline is highly volatile, in the event of its leakage from a storage tank, a large amount of vapor is rapidly generated from the surface of the gasoline and mixes with the air, forming a flammable gas mixture in the immediate surroundings. If the flammable gas mixture in an enclosure is ignited, the gasoline vapor burns explosively, causing extensive damage. Therefore, for risk management in a gasoline storage area, assuming a gasoline leakage accident, it is necessary to predict the fire hazard for the inflammable vapor and the explosion damage. The aim of this study is to obtain the knowledge necessary for the risk assessment of a gasoline storage area. A prediction model for the spread, evaporation, and diffusion behavior of leaked gasoline was proposed. The proposed model was verified by

conducting evaporative diffusion and ignition tests on leaked gasoline. Furthermore, a methodology was suggested for evaluating the explosion risk caused by vapor generated from leaked gasoline spread on the floor. The proposed method enables the prediction of the explosion damage in the event of gasoline leakage.

- **Keywords:** Gasoline leakage; Prediction model; Evaporation; Diffusion; Explosion damage

Abdul-Waris Dawuda, Mohammed Taleb-berrouane, Faisal Khan. *A probabilistic model to estimate microbiologically influenced corrosion rate*. Pages 908-926.

This work presents a new probabilistic methodology and model to estimate the microbiologically influenced corrosion (MIC) rate. The proposed methodology considers the variability of the corrosion causing parameters, complex interdependencies of the parameters, and updating the corrosion rate in response to evolving conditions. The proposed method is used to develop a fully parameterized Bayesian network model for the MIC rate. The model is tested using MIC field data. The results show that the metabolism of iron-oxidizing bacteria and methanogens are the most probable contributors to the corrosion rate. The study also identifies the most sensitive parameters affecting the corrosion rate. The proposed model plays a vital role in safety assessment and corrosion risk management of oil and gas production and processing assets.

- **Keywords:** Bayesian network; Predictive modeling; Sensitivity analyses; Microbiologically influenced corrosion; Corrosion rate; Biological corrosion

Boxi Shen, Zhijun Li, Xiangjin Kong, Mengliang Li, Zhenguo Li, Shijuin Shuai, Shiyu Liu. *Experimental and numerical investigations into effects of urea-water solution injection on tailpipe particulate matter emissions*. Pages 927-938.

Selective catalytic reduction (SCR) is currently the most effective method to control NOx emissions for heavy-duty vehicles. However, urea-water solution injection may lead to increase of particulate matter (PM) emissions. In this study, PM emissions caused by urea-water solution injection from a China VI heavy-duty vehicle under real-world driving conditions is investigated experimentally. Average PM number emissions increase by over 200 % due to urea-water solution injection. Inlet temperature and space velocity are found to be significant factors. Droplet depletion model is developed for analyzing the contribution of urea decomposition by-products. Results suggest that secondary-breakup-based particles is major contributor to particles formation instead of primary-breakup-based. About 20 % of secondary-breakup-based particles are nuclei mode particles and 80 % are accumulation mode particles. The main component of the secondary-breakup-based particles is cyanuric acid and ammelide.

- **Keywords:** Air pollution prevention; Diesel engine; Selective catalytic reduction; Particulate matter; Urea decomposition; Secondary breakup

Yang, Hongwang Jin. *Study on the combined effect of duct scale and SBC concentration on duct-vented methane-air explosion*. Pages 939-949.

A gas explosion is often vented to a safe location by means of a discharge duct. However, the presence of a discharge duct increases the explosion severity in the vessel, inducing a higher explosion overpressure compared to a simply vented vessel. To reduce the explosion overpressure in the vessel, an experimental study was performed to suppress the methane-air explosions in a 5 L vessel connected to a discharge duct of different scales (e.g., length and diameter) and with various sodium bicarbonate

concentrations. The results show that the initial flame propagation process in the vessel was basically similar in the simply vented vessel and in the vessel vented through a discharge duct (i.e., ducted-vessel). In the middle and late stages of flame propagation in the vessel, the flame fragmentation was more pronounced for the ducted-vessel. Moreover, the degree of flame fragmentation in the vessel increased with the duct length. The flame structure in the vessel was more irregular for a larger vent coefficient (Kv = 9.75). The more pronounced quenching in the short duct (250 mm duct) is related to the high inhibition efficiency due to the leakage of a large amount of sodium bicarbonate (SBC) powder into the discharge duct while in the long duct (750 mm duct) the disturbance is due to the strong turbulence. The appropriate SBC concentration can transform the mechanism for the pressure rise in the vessel. At high powder concentrations the maximum pressure in the vessel is dictated by the flame reaching the vessel wall, while at low concentrations the maximum pressure is dominated by the pressure (i.e., burn-up) in the discharge duct. There is an approximately linear correlation between the maximum pressure and the average flame velocity in the discharge duct for a given powder concentration, and a linear relationship between the maximum pressures in the vessel and the duct independent of the SBC concentration. Through the analysis of the flame dynamics (e.g. flame morphology, flame propagation velocity and turbulence) and friction resistance induced by the varying duct scales, the suppression efficiency of SBC powder in the vessel is higher for a longer and narrower discharge duct.

- **Keywords:** Gas explosion; Flame propagation; Explosion suppression; Ducted venting

Wissam H. Alawee, Suha A. Mohammed, Hayder A. Dhahad, A.S. Abdullah, Z.M. Omara, F.A. Essa. *Improving the performance of pyramid solar still using rotating four cylinders and three electric heaters*. Pages 950-958.

The world suffers from the potable water shortage problem. Solar still is a simple device used to convert the brackish water into a drinkable water. We proposed a new modification in the design of the pyramid solar still to enlarge the exposure area and decrease the depth of the water film as possible. So, four rotating cylinders were incorporated into the basin of the pyramid distiller. Also, three electric heaters were fixed on the basin water to raise its temperature. The energy required to run the heaters was captured from a PV system. The performance of the modified pyramid solar still with rotating cylinders (MPSSRC) was investigated under different rotating speeds (0.1, 0.2, 0.5, 1.0, 1.5, and 2.0 rpm). The experimental results revealed that the total distillates of the MPSSRC without heaters and reference still were 7300 and 3000 mL/m² a day, respectively with an improvement of 143 %. In addition, the total distillates of the MPSSRC with heaters and reference still were 9100 and 2900 mL/m² a day, respectively. So, the productivity was enhanced by 214 %. The optimum increase in productivity was obtained at the cylinders' speed of 0.5 rpm. The optimum thermal efficiency of the MPSSRC was obtained when using the electric heaters with the rotating speed of 0.5 rpm, where it was 65 % and 54 % for the MPSSRC with and without heaters, respectively.

- **Keywords:** Pyramid solar still; Drum; Solar distillation; Cylinder; Speed

Qingrui Shang, Supan Wang, Xuhai Pan, Shicheng Shi, Yuheng Ma, Juncheng Jiang. *Two-phase expanding mechanism and pressure response characteristic of boiling liquid expanding vapor explosion under rapid depressurization*. Pages 959-967.

The two-phase flow evolution, internal pressure, and thermodynamics responses during a BLEVE (boiling liquid expanding vapor explosion) process with water are assessed. Various initial pressures ranging from 1.7 to 5.7 barg, liquid fills load and different pressure relief ways were tested. Results show that after the pneumatic valve was opened, the rise velocity of the bubble increased first, and then decreased until the rupture or collision of the bubbles. The countercurrent flow reversed to the mainstream was experimentally observed and inhibited the expansion flow to reduce the boiling intensity. Thus, as the initial pressure increased, the average rate of pressure rose first increased, then slightly decreased due to the competitive effects of expansion flow and countercurrent flow. The interactions between the rarefaction wave driven by a sudden opening of a valve and the medium degree of superheat, control the pressure response, and the delay of boiling can be classified into the rarefaction wave control region ($dp/dt < 0$) and the superheat degree control regime ($dp/dt > 0$). And the effect of the liquid fill level on the rate of pressure rise was not affected by the countercurrent flow. The boiling explosion after the crack formed was intensified with pressure relief action caused by a separate piece of equipment, due to the enhanced heterogeneous boiling on the inner wall.

- **Keywords:** BLEVE; Pressure characteristic parameters; Thermodynamics; Two-phase flow; High-speed photography; Pressure relief action

Ana C. Spínola, Carolina T. Pinheiro, Abel G.M. Ferreira, Licínio M. Gando-Ferreira. *Mineral carbonation of a pulp and paper industry waste for CO2 sequestration*. Pages 968-979.

This study focuses on the mineral carbonation to capture CO2 using an alkaline industrial waste, the grits, formed during the kraft pulp production process. An indirect mineral carbonation route was adopted, composed by two steps: first the extraction of calcium from the grits and second the precipitation of calcium carbonate. Firstly, four solvents were analyzed (HNO3, CH3COOH, NaOH and NH4Cl). Only HNO3 and CH3COOH have shown significant extraction efficiencies of 79.4 and 73.2 %, respectively, after 2 h at 30 °C. Kinetic tests demonstrated that equilibrium conditions are reached after 60 min. Since the nitric acid is a corrosive acid and with high associated costs, the acetic acid was selected for the dissolution of grits and extraction of calcium. The optimal conditions determined were an acetic acid concentration of 2 M, solid/liquid ratio of 30 g/L and temperature of 45 °C with an efficiency approximately of 77 %. In the second step, carbonation experiments were performed contacting the Ca-rich liquor, obtained from the extraction step, with a flux of pure CO2 gaseous in a stainless inox reactor. The optimal conditions determined were 30 °C and 30 bar, reaching a carbonation efficiency of 74 %, corresponding a CO2 sequestration capacity of 460 kg CO2/ton of grits.

- **Keywords:** Mineral carbonation; CO2 sequestration; Alkaline waste; Grits; Experimental design

Zhenxin Jiang, Qingyan Chu, Haiyu Yang, RongRong Zhao, Yueman Yu, Ming Wang, Ransheng Liu. *Kinetic model for removing phosphorus and zinc from waste lubricating oil by pyrolysis*. Pages 980-991.

The present study focused on the establishment of a kinetic model for the removal of phosphorus and zinc from waste lubricating oil by pyrolysis. Zinc dialkyl dithiophosphate (ZDDP) was used as the model compound for the analysis. The pyrolysis of ZDDP was evaluated at different temperatures by infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy. Moreover, thermogravimetry (TG), derivative thermogravimetry (DTG), and differential scanning calorimetry (DSC) curves were used to investigate the thermal decomposition characteristics of ZDDP at different heating rates. The apparent activation energies at different conversion rates were calculated by the Kissinger–Akahira–Sunose (KAS) and Flynn–Wall–Ozawa (FWO) methods. Finally, the thermal

decomposition mechanism at each stage was determined by a model-based approach. The results indicated that the thermal decomposition process of ZDDP could be described by a four-step thermal decomposition model. The average apparent activation energy calculated by the FWO method was 107.959 kJ mol−1, while that calculated by the KAS approach was 105.0681 kJ mol−1. Additionally, it was established that the decomposition induction stage (II), competitive reaction stage (III), and precipitation stage (IV) involved a power function model reaction (P4) mechanism, Avrami–Erofeev reaction (A3) mechanism, and Avrami–Erofeev reaction (A2) mechanism, respectively. Importantly, the predactyl factor A and reaction rate constant K were also obtained. The outcomes of this study provide a valuable basis for optimizing the process of industrial pyrolysis of waste lubricating oil.

- **Keywords:** Waste lubricating oil; Zinc dialdehyde dithiophosphate; Thermal decomposition; Kinetics; Non-isothermal method

Krishnapandi Alagumalai, Ragurethinam Shanmugam, Shen-Ming Chen, Sivakumar Musuvadhi Babulal, Alagarsamy Periyalagan. *Novel electrochemical method for detection of cytotoxic Tinidazole in aqueous media*. Pages 992-1005.

Antibiotics drugs are essential pharmaceutical compounds that play a vital role in the pharmaceutical industry, hospital, and livestock farming. The large scale of pharmaceutical and husbandry effluents are the primary environmental pollutants in water bodies. Even low concentrations of toxic nitroimidazole residues could lead to severe issues for humans and aquatic environments. Simultaneously, electrochemical sensing of cytotoxic antibiotics provides a critical assurance in quality control laboratories, pharmaceutical industries, and in environment pollutant assessment. The electrode surface modification with an excellent electrocatalyst paves the way for the effective determination of these cytotoxic antibiotics. Herein, Noble metal silver incorporated carrom coin structured cobalt oxide (Ag-Co3O4 NPs) was synthesized through a simple co-precipitation technique, and its electrocatalytic actives sites were improved via calcination at 600°C. The modified electrodes were implemented in the electrochemical detection of cytotoxic Tinidazole (TNZ). The electrochemical characterization shows low charge transfer resistance (Rct) and prominent electrochemical active surface area (ECSA). Due to its unique properties, Ag-Co3O4 NPs modified glassy carbon electrode (GCE) exhibits excellent sensitivity, stability, reproducibility, and low detection level up to the Nanomolar scale. Further, it also provides excellent selectivity among other interfering drugs and species. Meanwhile, it paves strategies for the real-time monitoring of TNZ in biological, pharmaceutical, livestock and various wastewater samples which could paves way for effective application in electrochemical sensors.

- **Keywords:** Co-precipitation synthesis; Electrochemical sensors; Pollutants; Tinidazole; Real-time monitoring; Wastewaters

Harry Waudby, Sharif H. Zein. *A circular economy approach for industrial scale biodiesel production from palm oil mill effluent using microwave heating: Design, simulation, techno-economic analysis and location comparison*. Pages 1006-1018.

This paper examines a green approach to produce industrial-scale biodiesel from a palm oil mill effluent (POME) using Microwave Heating. Kinetic data were determined for this reaction and implemented into the Aspen HYSYS simulation software to produce an economic analysis of the process. It was found that the process is economically feasible with the inclusion of significant recycle streams and additional separation equipment. It was found that Malaysia might be the best location to repurpose palm oil mill effluent

(POME) because of palm oil production density. Thailand provides modest sea access and the best direct connection with mainland Asia, proving advantageous when distributing biodiesel fuel. Although Malaysia shares this connection to the mainland, terrestrial transport would have to travel a greater distance, increasing costs and emissions. Indonesia, however, offers the largest number of potential plant locations with direct sea access.

- **Keywords:** Biodiesel; Palm oil mill effluent (POME); Microwave heating; Techno-economic analysis; Simulation; Circular economy

Moshood Onifade, Bekir Genc, Abisola Risiwat Gbadamosi, Andrew Morgan, Thapelo Ngoepe. *Influence of antioxidants on spontaneous combustion and coal properties*. Pages 1019-1032.

Spontaneous combustion (SPONCOM) of coal is well known to be a serious threat to the safety of mineworkers, mining equipment and to the environment. It is also the biggest reason behind the coal mine fires. In this study, the influence of antioxidants on coal properties and SPONCOM liability of coal samples collected from South African coal mines was investigated. These antioxidants minimized SPONCOM but have effects on coal properties as confirmed under laboratory tests. As part of the design and test of a spray machine on two 60 T stockpiles using powdered gypsum as an antioxidant, the tests show an increase in the temperature distribution of the untreated stockpile compared to the treated stockpile. Gypsum, which has been used for the first time, proves to be an economically viable option compared to other antioxidants on both laboratory and medium-scale tests.

- **Keywords:** Antioxidant; Coal properties; Coalfields; Spontaneous combustion liability

Yangpeng Liu, Jiaxing Shen, Jing Ma, Guochun Li, Zihao Zhao, Xiaomin Ni, Xishi Wang. *Laser-based measurement and numerical simulation of methane-air jet flame suppression with water mist*. Pages 1033-1047.

Fire incidents caused by leaks from natural gas pipelines should be quickly controlled by using clean and efficient approaches, such as water mist. Previous studies on the methane-air jet fire suppression by water mist have paid not only little attention to the OH radical distribution characterizing the combustion intensity, but also critical extinguishing conditions of jet fires. Therefore, planar laser-induced fluorescence of the OH radical is obtained to visualize OH radical distribution in fire suppression. Fire Dynamics Simulator v 6.7.4 is applied to simulate the flame-spray interaction and detail the instantaneous fire-extinguishing process by the flow field, gas temperature, reaction methane mass fraction and radiation attenuation in non-lift-off jet flame scenarios. The results show that, considering variation of the jet flame tilt angle, the jet fires can be effectively suppressed when the gas-spray momentum ratio is below 0.0068 in non-tilted cases and normalized Reynold number is less than 2.56 in tilted cases. In the terms of water mist system optimization, the installation location of 1.45 times the pipe diameter was considered as the maximum nozzle horizontal position for fire suppression in the flame Froude number range of 0.2~1.5. Besides, the OH-PLIF measurement revealed that fire suppression resulting from the kinetics effect depends on whether the OH* flame structure is quickly broken by the downward spray thrust. This study may provide suggestions for natural gas fire suppression with water mist system, and give help for the reduction of greenhouse gas emissions under Paris Agreement.

- **Keywords:** Safety; Natural gas leakage; Fire suppression; Water mist; Fire dynamics simulator

Ning Ai, Sa Lou, Fengyan Lou, Chengda Xu, Qining Wang, Ganning Zeng. *Facile synthesis of macroalgae-derived graphene adsorbents for efficient CO2 capture*. Pages 1048-1059.

Graphene, emerging as one of the most promising class of adsorptive separation carbon material for its high specific surface area and strong surface chemical activity. Biomass especially sustainable biomass as graphene sources shows great potential at large scales under energy shortage era. In this paper, a kind of subtropical macroalgae (Sargassum Horneri, S.H.) was selected as the precursor, and a facile synthesis method based on KOH activation was used to prepare graphene. A continuous monitoring on the formation of graphene and a systematic investigation into biomass precursor were performed, paying special attention to parameters including activation temperature, the alkali and carbon ratio, the corresponding pore structure, and surface chemistry variation. Moreover, the CO2 adsorption properties of porous graphene were tested. The results showed that, S.H. is a kind of ideal graphene precursor. The optimum preparation of porous graphene by KOH activation was the carbonization temperature of 400 °C, the alkali carbon ratio of 4:1 and the activation temperature of 850 °C. The porous graphene displayed high specific surface area (~1411 m2/g), pore volume (~1.16 cm3/g), and abundant microporous and mesoporous structures. The as-prepared porous graphene exhibited good CO2 uptake capacity as 2.78 mmol/g at 30 °C and 1 bar. The CO2 adsorption rate equations of the graphene were consistent with the intraparticle diffusion model, indicating that the CO2 adsorption was mainly controlled by the pore structure, and additionally influenced by the chemical functional groups especially N on the surface.

- **Keywords:** Macroalgae; Graphene; KOH activation; CO2 adsorption

Humair Ahmed Baloch, M.T.H. Siddiqui, Sabzoi Nizamuddin, Sajid Riaz, Muhammad Haris, N.M. Mubarak, G.J. Griffin, M.P. Srinivasan. *Effect of solvent on hydro-solvothermal co liquefaction of sugarcane bagasse and polyethylene for bio-oil production in ethanol–water system*. Pages 1060-1069.

This study aims to investigate the role of water and ethanol in ethanol/water mixed solvent system, co-liquefaction of high-density polyethylene (HDPE) and sugarcane bagasse (SCB) to produce high quality bio-oil. It was revealed that various ethanol/water mixing ratios led to various reaction mechanisms, which indicates that there is a clear synergy effect between water and ethanol liquefaction process in three reaction media. The conversion and bio-oil yield approach were in the order of pure water < pure ethanol < water/ethanol mixed solvent regardless of the feedstock composition. Furthermore, detailed analysis of bio-oils was preformed such as CHNS/O analysis, chemical composition, 13C and 1H NMR analysis, higher heating value (HHV), TGA and FTIR analysis. The sugarcane bagasse-plastics derived bio-oil was found effective to enhance the qualitative properties of bio-oils compared from the pure sugarcane bagasse. The co-liquefaction of HDPE and SCB in mixed solvent was found more effective to enhance the qualitative and quantitative features of bio-oils compared to sole water and ethanol solvent.

- **Keywords:** Hydrothermal; Solvothermal; Mixed solvent; Supercritical fluids; HDPE; Bagasse

Qun Liu, Lu Li, Xiaoli Zhao, Kang Song. *An evaluation of the effects of nanoplastics on the removal of activated-sludge nutrients and production of short chain fatty acid*. Pages 1070-1076.

Nanoplastics in the environment and their effect on the ecosystem has aroused wide concern. This study investigated the effect of polystyrene nanoplastics on activated

sludge properties, including nutrient removal, dewaterability, and short chain fatty acid (SCFA) production potential. The results indicated that the nanoplastics inhibited the ammonia oxidation rate and nitrate generation rate during nitrification. The denitrification rate was also inhibited in the presence of nanoplastics, while the percentage of total inorganic nitrogen removed was not affected. The phosphorus absorption rates during the aerobic stage were 75.52 %, 76.19 %, 60.69 %, 71.58 %, and 49.48 % for nanoplastics concentrations of 0, 10, 50, 100, and 1,000 μg/L. The phosphorus release was inhibited in the reactors where nanoplastics were added during denitrification. These results indicate that bacteria, including nitrifiers, denitrifiers, and phosphorus-accumulating bacteria are affected by the nanoplastics. This probably attributed to the nanosize of the polystyrene effect on bacterial cells or overproduction of reactive oxygen species that caused dysfunction of microbial metabolism. SCFA production was inhibited by adding nanoplastics, particularly at a concentration of 10 μg/L, suggesting that the hydrolysis and acidification processes were affected by the nanosized polystyrene. The dewaterability of the activated sludge was improved after adding nanoplastics, this probably attributed to the aggregation of polystyrene and its function as a sludge skeleton builder. The results of this study reveal that nanoplastics have a negative effect on activated sludge properties, which should be considered for practical applications.

- **Keywords:** Nanoplastics; Nutrient removal; Short chain fatty acid; Polystyrene; Dewatering

Zhen Liu, Da-Ren Chen, Peng Wang, Zhongli Ji. *Effect of high pressure on the performance of coalescing filter cartridges for the natural gas purification*. Pages 1077-1089.

The performance of coalescing filter cartridges (of four different specifications) after a 410-day field operation for the high-pressure natural gas purification has been evaluated in this study. Our evaluation of field-tested filter cartridges showed the increase of the filter pressure drop by a factor of 5.28 and the decrease of the filtration efficiency at various degrees, resulting in 50.3 % loss in the filter quality factor (on average). The above evidenced the performance degradation of coalescing filter cartridges after the field application. Through the basic property characterization of composite media in tested filter cartridges, it was found the observed performance degradation of tested coalescing filter cartridges was attributed to the increase in the pore size of the coalescing layer (0.4–30.4 %), and the decrease of both pore size (2.3–23.7 %) and thickness (3.3–28.7 %) in the drainage layer. Via the performance evaluation of composite media composed of only coalescing and drainage layers used in both fresh and tested cartridges, it is concluded that the coalescing filter cartridges with composite media having both oleophobic coalescing and drainage layers, and high tensile and compression strengths, are excellent candidates for the stable and reliable operation of natural gas filtration at high pressure.

- **Keywords:** Natural gas filtration; High pressure operation; Coalescing filtration; Coalescing filter cartridges; Pore size

Niranjan Ravi, Daniel P. Johnson. *Artificial intelligence based monitoring system for onsite septic systems failure*. Pages 1090-1097.

An onsite sewage system (OSS) is a complex system that takes advantage of nature's biological processes to remove harmful pathogens from wastewater and reintroduces clean water back into the natural water cycle. However, the failure of an OSS can contaminate drinking water, surface water and release hazardous pathogen and chemicals creating hazardous conditions within the local environment. This research aims to provide an artificial intelligence (AI) solution using machine learning (ML) algorithms such as logistic regression (LR), random forest classifier, and K-nearest neighbors (KNN) to understand and examine the underlying factors that could cause septic failures. Septic

records from 1970 to 2019 were collected from five different counties across the State of Indiana and ML algorithms were applied to predict areas of possible septic failures. The algorithms demonstrated accuracy of approximately 80% in prediction of OSS failures. Such algorithms can assist state and county health departments in alerting homeowners of impending failures. Such an approach has the ability to not only prevent failures but also in the maintenance of a safe environment for communities reliant of OSSs. This approach was implemented and tested in the Indiana State Department of Health (ISDH).

R. Eyssette, F. Heymes, A.M. Birk. *Ground loading from BLEVE through small scale experiments: Experiments and results*. Pages 1098-1109.

The ground force generated by a BLEVE is a hazard that has been seldom studied, even though BLEVE has been source of many research works in the past decades. However, emergency responders have been asking questions the risk and consequences of a BLEVE on a bridge and other critical infrastructures for a while, with no answer so far. Moreover, a tank truck accident in Bologna in August 2018 has shown that bridge collapse may result from such scenario. This paper presents the experimental work done with a small scale apparatus reproducing realistic BLEVE failure with a cylindrical tube. Load cells were placed under the base plate holding the tube to measure the local ground force generated by the explosion. Forces from 10 kN to 55 kN were measured for a 50 mm diameter tube with 300 mm length failing at pressures from 10 to 32 Bar. The ground force signals are interpreted together with the imaging and internal pressure signal. The synchronization between violent boiling, repressurization in the vessel and strong ground force is clear through this comparison. Different ground force signals were observed depending on the fill level and weakened length of the tube. The maximum ground force and impulse vary almost linearly with failure pressure and liquid fill level. It is less clear for the influence of weakened/opening length of the tube. More data is required to conclude on this parameter influence.

- **Keywords:** Boiling Liquid Expanding Vapor Explosion; Explosion; High speed imaging; Explosive phase change; Failure analysis

Thanaphat Chukeaw, Worapinit Tiyatha, Kanticha Jaroenpanon, Thongthai Witoon, Paisan Kongkachuichay, Metta Chareonpanich, Kajornsak Faungnawakij, Nevzat Yigit, Günther Rupprechter, Anusorn Seubsai. *Synthesis of value-added hydrocarbons via oxidative coupling of methane over MnTiO3-Na2WO4/SBA-15 catalysts*. Pages 1110-1122.

Methane, the main component of natural gas and considered a greenhouse gas, was converted to value-added hydrocarbons (C2+) using synthesized Na2WO4 and MnTiO3 supported on SBA-15 through the oxidative coupling of methane. The MnTiO3 co-impregnated with Na2WO4 on SBA-15 (MnTiO3-NW/SBA-15) was more active than catalysts that were prepared using a simple one-pot impregnation of Mn2+, Ti4+, and Na2WO4 over fumed-SiO2, MCM-41, or SBA-15. Characterizations of the catalysts suggested that the presence of MnTiO3 was more important in the activation of methane relative to Mn2O3. The highest C2+ yield obtained from MnTiO3-NW/SBA-15 was 24.9 % with 63.0 % C2+ selectivity and 39.4 % CH4 conversion at a reaction temperature of 700 °C, a feed ratio of CH4:O2:N2 = 3:1:4, and a space velocity of 18,500 h−1. A time-on-stream test of MnTiO3-NW/SBA-15 over 25 h revealed that the C2+ yield slowly decreased from 24.9%–20.2% at the end of the 25 h run, because of a decrease in the catalyst's surface area, a loss of active Na2WO4 from the catalyst, and the destruction of α-cristobalite. Experiments using in-situ diffuse reflectance infrared Fourier transform spectroscopy with mass spectrometry, operated at 475 °C, revealed that the MnTiO3-NW/SBA-15 catalyst enhanced the formation of CH3 and H radicals, while no products or intermediates were found when only SBA-15 was tested.

- **Keywords:** MnTiO3; Na2OW4; Oxidative coupling of methane; SBA-15; Silica

Jiangang Zhao, Zhaoyou Zhu, Zhaoyuan Ma, Fei Zhao, Xiao Yang, Yinglong Wang, Peizhe Cui, Xin Li, Jun Gao. Double-column batch stripper process based on heterogeneous property and control strategy for the efficient separation of a ternary mixture containing two minimum boiling azeotropes. Pages 1123-1132.

Batch distillation is widely applied in the fine chemical industry due to the market demand for low-volume and high-value-added products. Heterogeneous ternary mixtures with two minimum boiling azeotropes, such as cyclohexane-acetonitrile-toluene, are common in production processes. However, the separation of a mixture based on batch distillation was rarely studied because of the complexity of the method. In this work, a double-column batch stripper (with a decanter) process with a processing capacity of 7200 kg was designed for the separation of a cyclohexane-acetonitrile-toluene ternary mixture by considering the heterogeneous properties of the components. The feasibility of the process was analyzed according to the phase diagram, and the production sequence was determined. The pressure of the columns and the decanter temperature were determined synthetically from the minimum total annual cost, operation time and recovery ratio. The production time of different components, which has significant impacts on the purity and yield, was determined. In view of the situation that two separated components would be successively obtained at the bottom of each column, a control strategy was designed which can switch the products vessels automatically and control the batch distillation process. The results show that the control structure exhibits a good controllability, and the purities of the separated products are all over 99.9 mol%. Based on the optimal batch distillation process, the environmental impacts of the process were calculated. The results of the environmental analysis show that the global warming potential (GWP), acid potential (AP) and human toxicity potential (HTP) are 8613.91 kg CO2 eq, 15.40 kg SO2 eq and 267.21 kg DCB eq, respectively.

- **Keywords:** Batch distillation; Control structure; Environment evaluation; Total annual cost; Binary azeotrope

Lidia Favier, Claudia Veronica Ungureanu, Andrei Ionut Simion, Gabriela Bahrim, Christophe Vial. *Enhancing the biodegradation efficiency of a emergent refractory water pollutant by a bacterial isolate through a statistical process optimization approach*. Pages 1133-1145.

Clofibric acid, the main pharmacologically-active metabolite of pharmaceutical products used as antilipaemic agent has received, in last years, an increased interest because of its well-known recalcitrance to biodegradation and its high persistence in the aquatic environment. This molecule passes unchanged or poorly transformed in wastewater treatment plants. An indigenous strain of Streptomyces, named MIUG 4.89 was previously selected, exhibited the ability to favor clofibric acid biodegradation within submerged cultivation in controlled biotechnological conditions. Thus, in order to enhance the biodegradation of this refractory molecule, mathematical modeling and statistical optimization designs associated to Plackett-Burman Design and Response Surface Methodology were used to evaluate and optimize the effects of different major culture conditions of this bacterial isolate. According to the results, under optimized culture conditions (5 g L−1 glucose, inoculation level 4.7 %, 27.5 °C and 20 days of incubation) the strain Streptomyces MIUG 4.89 exhibited a successful removal of clofibric acid with a biodegradation yield of 54 %, which is in agreement with model prediction. Thus, under optimized conditions, the removal yield was enhanced, which is very promising accounting for the refractory character of this water pollutant.

- **Keywords:** Clofibric acid; Streptomyces; Biodegradation; Plackett-Burman design; Response surface methodology

Meng Li, Jingcheng Liu, Huiqun He, Kanhua Su, Xiaole Guo, Weiqing Chen. *Safety and reliability evaluation of casing in ultra-deep well based on uncertainty analysis of extrusion load*. Pages 1146-1163.

The extrusion load on casing in ultra-deep well is uncertain, which limits the application of safety factor method. Therefore, the evaluation method of collapsing safety and reliability on casing during drilling in ultra-deep wells is put forward. Based on the extrusion load model in ultra-deep well considering the diversity of strength parameters of casing and the integrity of formation-cement sheath-casing system, the uncertainty distribution functions of collapse strength and extrusion load on casing are derived by introducing probability and statistics theory. Then, the theory of "stress-strength interference" is applied to obtain the reliability R, confidence interval and reliability-safety factor nR of casing. Taking multiple ultra-deep wells in the Kuqa block of the Tarim Oilfield as an example, the collapse safety and reliability analysis on casing is carried out. Several conclusions are made based on the oilfield statistics. The traditional safety factor is greater than the reliability-safety factor. The surface casing and the production casing are both safer than the technical casing. More accurate original data can narrow the confidence interval width of nR and reduce the collapse risk of technical casing. The change in reliability is consistent with the change of the reliability-safety factor. For technical casing, when R is greater than 0.50 and 0.92, nR is greater than 1.0 and 1.1 respectively. For production casing, when R is greater than 0.98, nR is greater than 1.1. For each type of casing, affected by the uncertainty of the extrusion load on casing, when the extrusion load exceeds a certain value (but this value is less than the casing strength), the reliability begins to decrease. The larger the standard deviation of extrusion load is, the more obvious the influence on reliability change will be. Compared with the traditional design safety factor, the change of the anti-collapse safety degree of the casing can be more intuitively displayed by the reliability, which could provide an important supplement for the selection of traditional design safety factor during drilling operations.

- **Keywords:** Ultra-deep well; Extrusion load; Uncertainty; Randomness; Reliability; Safety factor

Dongmei Huang, Chen Chen, Zhihao Xu, De Li, Long Shi, Guanghua Liang. *Fire behaviors of two-layer coated latex foam with an extremely thin surface layer under bottom ventilation conditions*. Pages 1164-1178.

Latex foam based upholstered furniture has been widely used in our daily lives. Its high fire risk can be reflected by its extremely thin surface layer together with a cellular structure sponge. Therefore, through this study, an experimental study was carried out to address the fire behaviors of typical latex foams, including cotton, hemp, silk, and blending coated latex foam. The thermal properties and structure of these fabric materials and latex foam were analyzed experimentally, together with the analysis of the heat transfer mechanism and the calculation of flame spread rate. Experimental results showed that the thin surface fabric covered on the surface of the latex foam could prolong the combustion process for more than 150 s. The peak bottom flame area of the silk coated sample was only 40 % of the uncoated one. The combustion residues of the surface fabric after the extinguishment were found composing of carbonized fabric and white ash. It was then known that the cotton fabric shows significant effects on the combustion processes due to dense residues. The average flame spread rate of the coated samples was about 22 % of those uncoated ones. The porosity of the fabric residues on the surface played a key role in the flame spread on the latex foam surface. A flame spread rate model was developed and validated for the first time that considered

the fabric porosity, which could provide a useful tool for the relevant fire risk evaluation for those practical fire scenarios with multi-layer combustible.

- **Keywords:** Two-layer coated latex foam; Fire behavior; Flame spread rate; Mass loss

Xiangkun Meng, Jingyu Zhu, Jiayue Fu, Tieshan Li, Guoming Chen. *An accident causation network for quantitative risk assessment of deepwater drilling*. Pages 1179-1190.

Quantitative risk assessment plays an important role in facilitating deepwater drilling safety. This paper proposes an accident causation network method for risk assessment during deepwater drilling. The method involves four basic steps: risk identification, failure scenarios definition, uncertainty evaluation, and accident path calculation. Risk factors regarding different sources such as the operator, process, equipment, and environment are firstly identified. Then a network topology based on graph theory models the underlying accident scenarios. Risk entropy is adopted to model the uncertain influence of multi-type risk factors. Dijkstra algorithm is finally used to calculate the shortest path from an initial event to a blowout accident. A deepwater drilling system is chosen as a case study to demonstrate the applicability of the proposed method. The result shows that changes of failure probabilities of risk factors lead to the variation of the shortest path both in probabilities and event sequences. With the assessment result, decision makers can take targeted measures to prevent accidents or reduce system risks.

- **Keywords:** Deepwater drilling; Quantitative risk assessment; Accident causation network; Risk entropy; Uncertainty modeling

Hemmat A. Elbadawy, Wagih A. Sadik, Amel F. Elhusseiny, Seham M. Hussein. *Design of economic photocatalytic system with low energy consumption, and high quantum yield, for the degradation of acid red 37 textile dye*. Pages 1191-1206.

This work aims to study the photocatalytic degradation of the textile dye pollutant, Acid Red 37, under UV irradiation in the bench scale batch photoreactor, designing an optimum system of nanometal oxides TiO2, ZnO and their mixtures with different weight ratios. The photocatalysts were synthesized and fully characterized by XRD, EDS and TEM. The photocatalytic degradation process was investigated as a function of pH, concentration of the dye pollutant and different ratios of the photocatalytic mixtures. Furthermore, the effect of adding electron scavengers; H2O2, Na2S2O8 and NaIO4 was studied. The best photodegradation was observed under UV irradiation upon adding a ratio of (3:1) (TiO2: ZnO) at pH = 6.5 when the textile dye concentration is 1.0 × 10−4 mol/L. The efficiency of the studied photocatalytic degradation systems can be arranged in the order: UV/ZnO < UV/TiO2< UV/TiO2/ZnO < UV/TiO2/ZnO/H2O2 < UV/TiO2/ZnO/ Na2S2O8 < UV/TiO2/ZnO/NaIO4. The system designated as UV/TiO2/ZnO/(1.1–5.5)x10-3M NaIO4 showed the highest photocatalytic degradation efficiency, with highest apparent quantum yield (11.1–16.6)% and the lowest electrical energy per order (37.0−22.2) kWh, indicating the lowest energy consumption relative to the other examined catalytic systems. Finally, these outcomes can be useful for photocatalysis with low depletion of electrical energy, greater amount of degradation and economical procedure.

- **Keywords:** Photocatalytic degradation; Nano metal oxides; Electron scavengers; Acid Red Dye 37; Electrical energy per order; Apparent quantum yield

Yanchao Li, Mingshu Bi, Yonghao Zhou, Zongling Zhang, Kai Zhang, Changshuai Zhang, Wei Gao. *Characteristics of hydrogen-ammonia-air cloud explosion*. Pages 1207-1216.

The main task of this work is to study the hydrogen-ammonia-air cloud explosion characteristics. The flame behavior and explosion pressure are obtained experimentally by changing equivalence ratio (ER) and ammonia fraction (AF). Then the correlation between flame behavior and maximum explosion pressure is revealed. Finally, the thermal, diffusion and chemical factors affecting laminar burning velocity (LBV) are analyzed. The results indicated that averaged flame propagation velocity (AFPV) and maximum explosion pressure (MEP), become decreased continuously with increasing AF, become increased firstly and then decreased with increasing ER. Maximum value of both AFPV and MEP of AF = 0.1, AF = 0.3, AF = 0.5 and AF = 0.7 is reached at ER = 1.4, ER = 1.2, ER = 1.0 and ER = 1.0. the MEP could be underestimated and overestimated by laminar and turbulent flame model. The MEP is largely affected by LBV especially when the flame instabilities are ignored. With increasing AF, the reduction of adiabatic flame temperature and thermal diffusivilty contributes to the LBV reduction. With increasing ER, the main factor affecting LBV is the generation and consumption of H radical.

- **Keywords:** Hydrogen-ammonia cloud explosion; Flame behavior; Maximum explosion pressure; Laminar burning velocity

Kazem Sarvestani, Omran Ahmadi, Seyed Bagher Mortazavi, Hasan Asilian Mahabadi. *Development of a predictive accident model for dynamic risk assessment of propane storage tanks*. Pages 1217-1232.

Investigation of past accidents has shown that LPG tank accidents cause significant damage to the industry due to the storage of large volumes of flammable materials in them. This study aimed for developing a predictive accident model for dynamic risk assessment of propane storage tanks of the refinery. Hazards and safety barriers were identified using MIMAH methodology. The basis of MIMAH methodology is Bow-tie method. To construct the Bow-tie diagram, first, accidents that occurred on LPG tanks were extracted from the databases of accidents and valid sources. The top events of the accidents were identified and analyzed by the fault tree. The Bow-tie diagrams were constructed and the barriers on the diagrams were identified and verified by refinery experts. According to the SHIPP model, safety barriers were categorized into seven main barriers. The failure rates of the fault tree basic events were extracted from reliable sources and the prior probability of barriers was calculated. Based on the failure or success of safety barriers, 6 levels of severity of consequences, safe, near miss, mishap, incident, and catastrophic accident were considered. Using the prior probability of failure of the barriers, the probability of occurrence of each level of severity of consequences was calculated with the event tree. In the next step, this paper employed LPG storage tanks past accidents to construct a likelihood function and update prior probability using the Bayesian equation. Finally, the posterior probability of occurrence of the consequences was calculated using the posterior probability of failure of the barriers. Because LPG accidents occur with low probability and high severity, predicting accidents dynamically helps people to always be prepared to prevent their occurrence.

- **Keywords:** Accident model; Dynamic risk assessment; LPG tank; MIMAH; Prior probability; Posterior probability

Chao Wei, Jianping Dong, Zehui Hu, Huining Zhang, Xu Wang, Zhifang Tong, Chunfa Liao. *CO2 sequestration exploration utilizing converter slag and cold-rolling waste water: The effect of carbonation parameters*. Pages 1233-1242.

The exploration of carbonation routine utilizing BOFs, CRW and CO2 has a significant effect on terminated treatment of metallurgical wastes resourceful disposal at a low cost. This paper investigated the collaborative effect of CRW composition on slag carbonation degree and CRW decalcification rate in CO2 sequestration system, furthermore, the effect of reaction time etc. on both were also discussed under optimal composition. Moreover, the carbonation process was simulated by Aspen software for comparing with the experimental results. The results showed that slag carbonation degree and CRW decalcification rate increased as CRW hardness increased, and kept stable. The optimal calcium conversion was 50.4 %, corresponding to 15.9g CO2/100g slag, and the decalcification rate was 87.1 %, respectively, at 80 °C and 10 L/kg for 60 min. The Aspen simulation results showed the correlation degrees were 0.94 for calcium conversion and 0.98 for decalcification rate.

- **Keywords:** CO2 sequestration; Converter slag; Cold-rolling waste water; Aspen simulation

Qiming Huang, Shimin Liu, Bing Wu, Gang Wang, Guofu Li, Zhiguo Guo. *Role of VES-based fracturing fluid on gas sorption and diffusion of coal: An experimental study of Illinois basin coal*. Pages 1243-1253.

As a kind of environmentally friendly and non-polluting fracturing fluid, the VES-based fracturing fluid is gradually promoted in the field coalbed methane (CBM) stimulation in recent year. However, the fracturing fluid residue trapped in the reservoir may have a potential negative impact on gas flow in CBM reservoirs. In this study, the fracturing fluid based on surfactant was selected to treat the coal sample. The lab experiments have been conducted including the isothermal methane sorption, the low-temperature nitrogen sorption and the 13C nuclear magnetic resonance (NMR) measurements. The results showed that the methane sorption capacity was modified with cleaning fluid treatment and residuals. It was found that the sorption capacity can be recovered through water washing. It is important to point out that the diffusivity of coal has been significantly damaged indicated by the paramount decrease of diffusion coefficient even after the water washing. Additionally, no significant chemical coal molecular structure changes were observed with VES-based fracturing fluid treatment based on the NMR data. The fracturing fluid changes the coal pore structure mainly because the residue of the fracturing fluid enters the coal pore system, thereby adhering on the pore wall or blocking the pore throat. Most residues entered into the coal seam will be trapped in mesopores and macropores, cause serious damage to the CBM diffusivity in the coal matrix, thereby posing an adverse effect to the CBM production.

- **Keywords:** Viscoelastic surfactant; Fracturing fluid; Sorption; Diffusion; Pore structure

Majid Saidi, Hossein Kadkhodayan. *Process development for sodium permanganate production by waste management of industrial sludge of zinc oxide ores recovery plants: Experimental and simulation study*. Pages 1254-1263.

Produced sludge in the hot refining stage of zinc oxide ores recovery plants contains huge amount of MnO2. Aspen Plus modeling assembled based on Taguchi experimental design has been utilized to study a new plan for sodium permanganate (NaMnO4) production from an industrial sludge containing MnO2. The optimized results by Taguchi approach has been applied as the initial data for the modeling and sensitivity analysis of process using Aspen Plus software. The influence of key operating factors such as acid concentration of electrolysis spent solution (CSE) in the range of 60−90 g/l, reaction temperature (TR) in the range of 70−100 °C, stirring speed of solution (S) in the range of 100−400 rpm, reactions time (τ) with value of 1−3 h, MnO2 content in the industrial

sludge (WMnO2) with values of 10–30 %, solid to liquid ratio (S/L) with amounts of 1:1−1:4, additives amounts (WAdditives) with values of 5−20 wt.% and oxygen gases pressure (PO2) in the range of 1–2.5 at m have been studied on the production efficiency of NaMnO4. The optimum condition to maximize NaMnO4 production from the industrial sludge has been found as: CSE=80 g/L, TR = 100 °C, S=300 rpm, τ=2.0 h, WMnO2 = 8 wt.%, S/L ratio = 1:2, WAdditives = 20 wt.% and PO2 = 2.5 atm. The maximum NaMnO4 production during designed process at optimized condition was more than 70 %. Also, under optimum condition, zinc extraction efficiency and removal percentage of Fe2+, Co2+, Mn2+ impurities from the industrial sludge were more than 85 % and 95 %, respectively.

- **Keywords:** Sodium permanganate; Industrial sludge of hot refining; Electrolysis spent solution; Aspen plus simulation; Taguchi approach

Peter Schmitz, Genserik Reniers, Paul Swuste, Karolien van Nunen. *Predicting major hazard accidents in the process industry based on organizational factors: A practical, qualitative approach*. Pages 1268-1278.

OCI Nitrogen seeks to gain knowledge of (leading) indicators regarding the process safety performance of their ammonia production process. The current sub-study raises the question whether major hazard accidents in the ammonia production process can be predicted from organizational factors, also called management delivery systems. This paper links organizational factors to accident processes and their barrier systems, using the bowtie metaphor. It is shown that organizational factors indirectly impact accident processes as they strongly influence the quality or trustworthiness of the barrier systems. By putting the right focus on organizational factors during audits or reviews, major accident processes get the attention they deserve, and the necessary actions are taken at the right management level. Qualitative and quantitative monitoring of organizational factors can provide a picture of their operation and efficiency. Using an example on retrospective data it is demonstrated that information from organizational factors could have stopped the development of the near-accident prematurely. However, organizational factors should first be qualitatively assessed before they are quantitatively monitored. A quantitative assessment has been worked out for one of the management delivery systems so to provide an example of management indicators. Determining these (management) indicators from threshold values is an intricate matter due to the complicated influence of organizational factors on accident processes, and requires more follow-up research.

- **Keywords:** Delivery systems; Safety management system; Process safety; Indicator; Ammonia; Organizational factors

Zuzhen ji, Shuang-Hua Yang, Yi Cao, Yuchen Wang, Chenchen Zhou, Liang Yue, Yinqiao Zhang. *Harmonizing safety and security risk analysis and prevention in cyber-physical systems*. Pages 1279-1291.

Cyber-physical system (CPS) has been widely adopted in modern industrial productions. Safety and security (S&S) play an important role in CPS, which assists the reliability of the system. Traditionally, safety and security risks were managed independently. As the development of cyber technology, S&S issues become complex and could affect each other in multiple ways. There is a strong need to develop a systematic method to manage safety and security risks simultaneously. In this work, a systematic method to integrately analyze S&S risks is proposed. Firstly, attack route models (ARM) as the root cause of typical cyber-threats are summarized from the literature together with their corresponding consequences in CPS. Secondly, in addition to commonly adopted physical safety prevention route (PSPR), cyber security prevention route (CSPR) based on ARM is

developed to investigate the safety hazards and security threats. Then, safety critical variable analysis (SCVA) is proposed to quantify the S&S risk. Finally, SCVA, CSPR and PSPR are integrated via the bowtie method. The key contribution of the work is the method which simultaneously consider safety and security risk for CPS. In parallel. SCVA represents the working status of CPS devices, which would be useful to quantitatively determine the severity of consequence and further level of risk.

- **Keywords:** Cyber-physical system; Safety and security risks; Risk assessment; Bowtie analysis; Safety critical variable

Hao Sun, Haiqing Wang, Ming Yang, Genserik Reniers. *Towards limiting potential domino effects from single flammable substance release in chemical complexes by risk-based shut down of critical nearby process units*. Pages 1292-1303.

The explosion load is a significant escalation factor possibly influencing the potential occurrence of domino accidents in chemical plants. It is not economical to install explosion isolation systems (e.g., extinguishing barrier) for all equipment or process units across a chemical plant. Although shutting down all equipment or process unit can prevent an explosion, it may also cause further economic losses. To prevent domino accidents, the process unit that needs to be shut down accurately should be selected, and the normal operation of other units needs to be ensured. A method to select the process unit to be isolated based on the Dimensioning Accidental Load (DAL) is proposed. By calculating the occurrence probability and consequences of the accident scenarios, the DAL of the surrounding units is determined. DAL is used as the impact intensity of the accident unit on the surrounding units. The probit model is used to calculate the damage probability of surrounding units. The case analysis results show that the method of selecting the process unit to be isolated based on DAL quantifies the impact intensity of the exploded unit on surrounding units from probability and consequence. Under the premise of meeting the acceptable risk criteria, the method can determine which units should be shut down and which units can operate normally when a release accident occurs. While preventing domino accidents, economic losses caused by the shutdown of all process units are reduced and a theoretical basis for accident prevention and safe operation of the plant is provided.

- **Keywords:** Safety; Vapor cloud explosion; Domino accident; Dimensioning accident load

Zohreh Rahimi-Ahar, Mohammad Sadegh Hatamipour. *Performance evaluation of a solar and vacuum assisted multi-stage humidification-dehumidification desalination system*. Pages 1304-1314.

This study compares the freshwater productivity of a three-stage vacuum humidification-dehumidification (VHDH) desalination system to a single-stage VHDH system. Experimental study on a multi-stage humidification in sub-atmospheric pressure condition confirmed its superiority over previous multi-stage humidification-dehumidification processes. The variation of the desalination rate was measured experimentally using the three-stage vacuum humidification and heating modes. The results showed that the maximum desalination rate of the unit was 1.8 kg.h−1 per 1 m2 of solar water heater area with minimum specific power consumption (SPC) of 0.1 kW h.kg−1 when the maximum solar intensity was 1106 W.m-2 in July 2020. This investigation indicated that the system had high freshwater productivity and low SPC compared to a single-stage VHDH system. The system performance was improved when the operation was further optimized using the response surface methodology (RSM). The optimal values of saline water to air mass flow rate ratio (sw/a) and humidifier pressure (PH) of 1.77 and 33 kPa led to the maximum freshwater productivity. In all operating

conditions, through converting the single-stage humidification to two-stage and three-stage humidification processes, the humidity ratio was enhanced by about 51 % and 19 %, respectively. The optimal freshwater productivity could be realized only when multi-stage vacuum humidification was utilized at isothermal heating mode in all stages and the cost was $0.002 per liter.

- **Keywords:** Multi-stage; Vacuum humidification; System performance; Desalination rate; Specific power consumption

S.K. Singh, Prabhat Vashistha, Ramesh Chandra, Anand K. Rai. *Study on leaching of electric arc furnace (EAF) slag for its sustainable applications as construction material*. Pages 1315-1326.

The steel production generates approximately 10 % of electric arc furnace slag on the production of each ton of steel. In the view of environmental concerns and government regulations regarding slag disposal, alternate ways of its utilization are required. This work is focused on the leaching behaviour study of electric arc furnace (EAF) slag to assess its suitability as construction material. EAF slag contains toxic metals; consequently, their leachable quantity may affect the eco-system. Chromium (Cr), lead (Pb), mercury (Hg), molybdenum (Mo) and cadmium (Cd) have found special concern due to their high toxicity for human kind as well as for the environment. The leaching study of EAF slag was carried out through the application of sequential batch water leaching tests (SWLT), batch test and toxicity characteristics of leaching procedure (TCLP) method. Fresh EAF slag was characterized by XRF, XRD, SEM and ICPMS analysis for the determination of essential compositions and contamination. SWLT was performed at different pH of 4.0, 5.3, 6.1, 7.2 and 8.5. It was found that toxic metals was not leached beyond permissible limits at any pH. Moreover, TCLP method was applied for the leaching analysis of EAF slag at pH of 4.93 and 2.88. The concentrations of toxic metals in leachates were found negligible through ICP-OES analysis. The batch test method was also applied upto 60 days of EAF slag. This test was carried out at various pH ≈ 4, 5 and 6. The obtained leachates were tested at 10 days, 15 days, 30 days, 45 days and 60 days of leaching. The ICP-OES analysis of leachates showed negligible concentrations of leached metals/elements. Through the application of different leaching test methods, it was found that the leaching of hazardous heavy metals from EAF slag is negligible or within permissible limits as per IS 383−2016 and EPA. Therefore, EAF slag can be utilized as construction material in eco- friendly manner.

- **Keywords:** Batch method; EAF slag; Environmental remediation; Hazardous element; Leaching behaviour; Sequential batch water-leaching tests; Sustainable utilization; TCLP method

Dongdong Yang, Guoming Chen, Jianmin Fu, Yuan Zhu, Ziliang Dai, Lei Wu, Jian Liu. *The mitigation performance of ventilation on the accident consequences of H2S-containing natural gas release*. Pages 1327-1336.

Ventilation is an available measure to dilute the released toxic gas and has been widely applied in offshore facilities to mitigate the adverse impact. However, "available" is never the same as "effective". Up to now, the mitigation performance of ventilation remains a challenging topic that needs to be further studied. To identify the effectiveness of the mitigation, a systematic approach is proposed concerning the toxic impact caused by the diluted toxic gas, during which the emergency evacuation is considered. The grid-based concept is adopted to identify the initial position with the worst toxic impact. Then the effectiveness of ventilation is estimated according to its ability on mitigating the worst toxic impact. Taking an offshore platform as a case, the toxic impact under different H2S leakage scenarios are predicted. The dependencies among the wind speed, leakage rate, concentration of H2S, and toxic impact are discussed. Some safety-related results can be obtained, such as accident scenarios where ventilation can effectively mitigate the toxic

impact. The present work could provide guidance to improve the safety of design and emergence plans in H2S release accidents.

- **Keywords:** Ventilation; Mitigation performance; Effectiveness; Diluted H2S; Emergency evacuation; Offshore platforms