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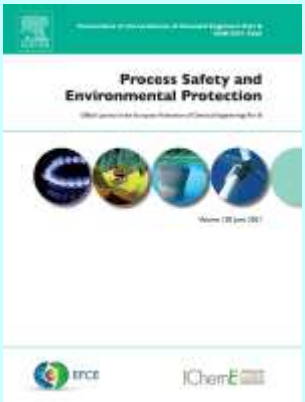

H. Sharon. ***Energy, exergy, environmental benefits and economic aspects of novel hybrid solar still for sustainable water distillation*****. Pages 1-21.**

In this work, a novel hybrid solar still which occupies less ground area has been proposed and investigated under the climatic conditions of Chennai, India. Hybrid solar still is formed by integrating basin solar still and vertical diffusion still. The proposed unit has been thermodynamically modeled and the effect of area ratio of basin to vertical absorber, diffusion gap, basin water depth, shade and feed water flow rate on unit's performance has been investigated. Optimum vertical diffusion still absorber area to basin area ratio, diffusion gap, basin water depth and feed water flow rate are found to be 2.0, 0.02 m, 0.02 m and two & half times the condensate production rate in vertical diffusion solar still, respectively. Shading of vertical absorber is found to decline the overall condensate production rate in a rapid manner. Exergy efficiency, exergy destruction and improvement potential of each component of hybrid solar still for all months has also been reported. The hybrid solar still is found to have high performance in winter seasons rather than summer seasons. Maximum condensate productivity rate, thermal and exergy efficiency of the optimized hybrid solar still is about 13.79 kg/d, 56.17 % and 6.93 %, respectively. Condensate production cost per litre ranges between 1.10 INR/L to 3.83 INR/L depending on wick replacement frequency, interest rate and life span of the unit. Energy payback time and finance payback time of the unit is within 1.2 Year and within 4.0 Year, respectively. Net CO2 emission, SO2 emission and NO emission mitigated by the unit ranges between 23.4–63.1 tons, 168.0–453.8 kg and 68.6–185.6 kg, respectively. Reasonable condensate production rate with acceptable price and environmental benefits has made this proposed still more promising for practical applications.

- **Keywords:** Hybrid solar still; Potable water; Thermodynamic analysis; Enviro-economic analyses; Solar energy

Yuzhuo Wang, Yingjie Li, Chunxiao Zhang, Liguo Yang, Xiaoxu Fan, Leizhe Chu. ***A study on co-pyrolysis mechanisms of biomass and polyethylene via ReaxFF molecular dynamic simulation and density functional theory*****. Pages 22-35.**

Co-pyrolysis of biomass and waste plastics is a long-term strategy to achieve efficient waste management and generate valuable fuels. The cellulose and polyethylene were chosen as typical representatives for biomass and plastics in this work. Reactive force field molecular dynamic and density functional theory were employed to investigate the co-pyrolysis mechanism of cellulose and polyethylene which were not readily achieved only by experiments. The hydrocarbon and H radicals from polyethylene respectively interact with the alcoholic groups and furans which contributes to producing alcohols and suppresses the generation of aldehydes and ketones. The energy barriers of rate controlling steps for producing long-chain alcohols (about 669.40 kJ/mol) in co-pyrolysis of cellulose and polyethylene are obviously smaller than those for producing oxy-compounds in cellulose pyrolysis alone. The formations of furan alcohols are easy with low energy barriers (22.19, 16.40 and 22.66 kJ/mol, respectively) in the presence of polyethylene. The co-pyrolysis of cellulose and polyethylene also promotes the formation of CH. The polyethylene has a positive effect on the improvement of major co-pyrolysis products. The reactive force field molecular dynamic simulation and density functional theory seems promising to determine the co-pyrolysis mechanisms of biomass and waste plastics at microcosmic level and help to produce high-quality fuels.

- **Keywords:** Waste plastics; Biomass; Co-pyrolysis; ReaxFF molecular dynamic; Density functional theory

Khuram Maqsood, Abulhassan Ali, Rizwan Nasir, Aymn Abdulrahman, Abdullah Bin Mahfouz, Anas Ahmed, Azmi B.M. Shariff, Saibal Ganguly, Muhammad Mubashir, Pau Loke Show. *Experimental and simulation study on high-pressure V-L-S cryogenic hybrid network for CO2 capture from highly sour natural gas*. Pages 36-50.

Cryogenic carbon dioxide (CO2) capture technologies showed promising results for the purification of highly sour natural gas reserves. However, quantitative experimental data for solid and liquid CO2 formation during cryogenic separation is not adequately examined in the previous studies. Moreover, an economical and efficient cryogenic CO2 capture technology with reduced energy and hydrocarbon losses is necessary to make it attractive for commercial use. A high-pressure cryogenic hybrid network comprised of the packed bed and the cryogenic separator was developed for the cryogenic experimental study on CO2 capture from binary CO2−CH4 mixture to focus these areas. Feed containing 30, 50 and 70 % CO2 content were used and the separation study was conducted in vapor-solid (V-S), vapor-liquid (V-L), and vapor-liquid-solid (V-L–S) regions of phase equilibria. The packed bed was used in the V-S operational domain to quantify CO2 solid up to 20 bar because of the operational limitations. Separation characteristics and V-L isothermal flash measurements at 20, 30, and 40 bar pressure and temperature ranges from -20 to −60 °C were carried out in the cryogenic separator. The operation in the setups was carried out at different compositions of the CH4−CO2 binary mixture to define the boundaries of the hybrid cryogenic network. Liquid formation at 40 bar for 70 % CO2 feed was 0.15 kg at -55 °C as compared to 0.03 kg for 30 % CO2 feed. The simulation study was carried out using Aspen Plus along with the Peng Robinson Equation of State (EoS), and the results were compared with the experimental data, which showed good agreement. The hybrid cryogenic network showed an energy reduction of 37 % compared to the conventional cryogenic distillation network with 90.6–97.3 % CH4 purity and 2.65–12.39 % methane losses with different arrangements of the hybrid cryogenic network.

- **Keywords:** CO2 capture; Separation characteristics; Hybrid cryogenic network; Solid quantification

Mohd Umair Iqbal, Mohammed Aatif Shahab, Mahindra Choudhary, Babji Srinivasan, Rajagopalan Srinivasan. *Electroencephalography (EEG)*

***based cognitive measures for evaluating the effectiveness of operator training*. Pages 51-67.**

Process industries rely on effective decision-making by human operators to ensure safety. Control room operators acquire various inputs from the DCS, interpret them, make a prognosis, and respond through appropriate control actions. In order to perform these effectively, the operator needs to have appropriate mental models of the process. Poor mental models would increase the operator's cognitive workload and make them prone to errors. Traditionally, operator training systems are used to help operators learn appropriate mental models. However, performance assessment metrics used during training do not explicitly account for their cognitive workload while performing a task. In this work, we demonstrate that this leads to an incorrect assessment of operators' abilities. We propose an Electroencephalography (EEG) power spectral density-based metric that can quantify the cognitive workload and provide detailed insight into the evolution of the operator's mental models during training. To demonstrate its utility, we have conducted training experiments with ten participants performing 438 tasks. Statistical studies reveal that the proposed metric can quantify the cognitive workload and therefore be used to assess operator training accurately.

- **Keywords:** Training; Operator performance; Mental model; Cognitive workload; Clustering

Hanling Mao, Siyue Li, Shun Lan, Shanshan Guo, Yuefeng Huang, Zhenfeng Huang, Xinxin Li, Xiaokang Li. *Uniform flow field design in porous media filter tower and experimental verification*. Pages 68-78.

Filter tower is usually used in industrial wastewater. However, filtration efficiency will be decreased because of the bias flow in filter tower. This paper is to propose a design method of uniform flow field in porous media filter tower. Firstly, based on the RNG k-ε turbulence model, porous media filter tower model is built and the computational fluid dynamics (CFD) is employed to simulate the flow field. The simulation results show that the throttle plate can make the flow field of the filter tower uniform. Secondly, in order to further study the flow field in filter tower, the optimal parameter combination of filter tower is obtained by monofactor analysis and orthogonal analysis. Finally, the optimal design parameters are verified by experiments. The simulation and experimental results show that the uniform flow field design method used in porous media filter tower is feasible.

- **Keywords:** CFD; Turbulent model; Adsorption efficiency; Optimization; Filter tower

Shi-Chun Xu, Yi-Feng Zhou, Chao Feng, Jing-Nan Zhang. *The factors of regional PM2.5 emissions inequality in China*. Pages 79-92.

Since the reform and opening up, China's economy has developed rapidly, which has also caused environmental problems such as industrial emissions. PM2.5 (particulate matter with a diameter of less than 2.5 microns) emissions seriously threaten people's health. Therefore, it is necessary to study the emission reduction of PM2.5. This study combines the Data Envelopment Analysis (DEA) and Logarithmic Mean Divisia Index (LMDI) methods to originally construct the inequality indicator and explore the influence of different factors on the inequality of per capita PM2.5 from the regional aspect. This study decomposes the "emission efficiency" of per capita PM2.5 emissions into more important effects. It reveals that, in East China, the energy-oriented technology gap (ETG) had the strong reducing effect on the national per capita PM2.5 emissions; the energy-oriented technology efficiency (ETE) and economic development level (EDL) had the strong promoting effect. In Central China, the potential emission intensity (PEI) has the strong reducing effect on the national per capita PM2.5 emissions, followed by the

EDL; the ETG and energy-biased technology (EBT) effect had the strong promoting effect. In West China, the ETE had the strong reducing effect on the national per capita PM2.5, followed by the PEI; the ETG had the strong promoting effect, followed by the EBT and output-oriented technology gap (YTG). The ETE had the greatest improving effect on the inequality indicator, and the PEI and EDL had the greatest reducing effect. Policy suggestions are put forward based on regional differences in East China, Central China and West China.

- **Keywords:** Inequality indicator; Decomposition analysis; DEA-LMDI method

Deyang Wu, Jinsong Zhao. *Process topology convolutional network model for chemical process fault diagnosis*. Pages 93-109.

There always exists potential safety risk in chemical processes. Abnormalities or faults of the processes can lead to severe accidents with unexpected loss of life and property. Early and accurate fault detection and diagnosis (FDD) is essential to prevent these accidents. Many data-driven FDD models have been developed to identify process faults. However, most of the models are black-box models with poor explainability. In this paper, a process topology convolutional network (PTCN) model is proposed for fault diagnosis of complex chemical processes. Experiments on the benchmark Tennessee Eastman process showed that PTCN improved the fault diagnosis accuracy with simpler network structure and less reliance on the amount of training data and computation resources. In the meantime, the model building process becomes much more rational and the model itself is much more understandable.

- **Keywords:** Fault diagnosis; Chemical process; Process topology convolutional network; Explainable deep learning; Process safety

Md. Tanjin Amin, Faisal Khan, Salim Ahmed, Syed Imtiaz. *A data-driven Bayesian network learning method for process fault diagnosis*. Pages 110-122.

This paper presents a data-driven methodology for fault detection and diagnosis (FDD) by integrating the principal component analysis (PCA) with the Bayesian network (BN). Though the integration of PCA-BN for FDD purposes has been studied in the past, the present work makes two contributions for process systems. First, the application of correlation dimension (CD) to select principal components (PCs) automatically. Second, the use of Kullback-Leibler divergence (KLD) and copula theory to develop a data-based BN learning technique. The proposed method uses a combination of vine copula and Bayes' theorem (BT) to capture nonlinear dependence of high-dimensional process data which eliminates the need for discretization of continuous data. The data-driven integrated PCA-BN framework has been applied to two processing systems. Performance of the proposed methodology is compared with the independent component analysis (ICA), kernel principal component analysis (KPCA), kernel independent component analysis (KICA), and their integrated frameworks with the BN. The comparative study suggests that the proposed framework provides superior performance.

- **Keywords:** Process monitoring; Fault diagnosis; Process safety; Correlation dimension; Vine copula; Bayesian network

Md. Tanjin Amin, Faisal Khan, Salim Ahmed, Syed Imtiaz. *Risk-based fault detection and diagnosis for nonlinear and non-Gaussian process systems using R-vine copula*. Pages 123-136.

This paper presents a risk-based fault detection and diagnosis methodology for nonlinear and non-Gaussian process systems using the R-vine copula and the event tree. The R-

vine model provides a multivariate probability that is used in the event tree to generate a dynamic risk profile. An abnormal situation is detected from the monitored risk profile; subsequently, root cause(s) diagnosis is carried out. A fault diagnosis module is also proposed using the density quantiles, developed from marginal probabilities. The performance of this methodology is benchmarked using the Tennessee Eastman chemical process. The proposed risk-based framework has also been applied to an experimental setup and a real industrial isomer separator unit. The diagnosis module is found sensitive to both single and simultaneous faults. The results confirm that the proposed methodology provides better performance than the conventional principal component analysis and transfer entropy-based fault diagnosis techniques using the advantage of marginal density quantile analysis.

- **Keywords:** Process safety; Risk assessment; Process monitoring; Fault diagnosis; R-vine copula

Mohammad Hossein Keshavarz, Zeinab Shirazi, Parvin Kiani Sheikhabadi. *Risk assessment of organic aromatic compounds to Tetrahymena pyriformis in environmental protection by a simple QSAR model*. Pages 137-147.

A new Quantitative Structure-Activity Relationship model is introduced for reliable prediction of the toxicity of organic aromatic compounds based on the logarithm of 50 % growth inhibitory concentration of Tetrahymena pyriformis (log(IGC50−1)), which have extensive use in ecotoxicology and environmental safety applications. The largest experimental data set of log(IGC50−1) for 892 organic aromatic compounds is used to derive and test the new model. A core correlation based on additive variables is introduced by the number of nitro groups, carbon and halogen atoms as well as some specific polar groups and molecular weight. An improved correlation based on two non-additive correcting functions is developed for the increment of the reliability of the core correlation. The reliability of the improved correlation is tested and compared with two of the best available methods, which require complex descriptors. The predicted results for 661 and 231 of training and test sets have been confirmed by internal and external validations. The values of correlation coefficient (R2), mean error (ME), root mean squared error (RMSE), and maximum of errors (Max Error) for 661/231 of training/test aromatic compounds are 0.8442/0.7771, 0.0000/0.0149, 0.3166/0.3603, and 0.9732/0.9825, respectively, which are good results as compared to extra complex models with lower reported data. Various statistical parameters confirm the goodness-of-fit, high reliability, precision, and accuracy of the novel model.

- **Keywords:** Toxicity; Tetrahymena pyriformis; Organic aromatic compound; Molecular structure; QSAR

Mohamed M.Z. Ahmed, Fuhaid Alshammari, A.S. Abdullah, Mohamed Elashmawy. *Basin and tubular solar distillation systems: A review*. Pages 157-178.

Both basin and tubular solar stills have been used for solar desalination for long time. Using solar energy for the freshwater production is a big challenge due to their low productivity with relatively high cost. However, in some specific situations like rural and isolated areas, it is considered suitable. The present study aims to analyze the latest situation of the solar water desalination based on the two typical solar stills (basin and tubular). The potential of both types for leading the future development of the solar desalination has been evaluated. Various techniques and developments of solar stills such as multi-effect, wick, heat storage materials, condenser surface and photovoltaic thermal (PVT) systems and atmospheric water harvesting (AWH) have been reviewed.

The most promising solar still techniques and the future expectations have been discussed at the end of the study.

- **Keywords:** TSS; Solar desalination; Multi-effect; PCM; Nanoparticles; Parabolic concentrator; AWH

Yanfu Wang, Kun Wang, Tao Wang, Xi Yan Li, Fasial Khan, Zaili Yang, Jin Wang. *Reliabilities analysis of evacuation on offshore platforms: A dynamic Bayesian Network model*. Pages 179-193.

An offshore platform is naturally vulnerable to accidents, such as the leakage of dangerous chemicals, fire and explosion. Oil and gas are explosive and all the equipment and pipes are squeezed into a limited area on a platform. Escape, Evacuation, and Rescue (EER) plans play a vital role as the last barrier to ensure the safety of personnel in the event of a major accident. As a result, the main contributors leading to evacuation failure need to be analyzed to prioritize technology development and select a robust EER strategy. This research aims to undertake the quantitative reliability analysis of various EER strategies on offshore platforms. First, a reliability prediction model of emergency evacuation is established for offshore platforms based on the K2 structure learning algorithm and a Bayesian network parameter learning method. The conditional probability table of each node is determined by combining the Bayesian estimation method and a junction tree reasoning engine. The reliability of emergency evacuation on a platform is predicted using a dynamic Bayesian network model. The transition probability is determined through a Markov method. The main factors leading to evacuation failure are investigated using the diagnostic reasoning method of Bayesian Network. The findings can provide insights for the development of cost effective EER strategies for an offshore platform.

- **Keywords:** K2 algorithm; Dynamic Bayesian network; Reliability prediction of successful evacuation; Analysis of influencing factors

Soumava Boral, Sanjay K. Chaturvedi, Ian Howard, V.N.A. Naikan, Kristoffer McKee. *An integrated interval type-2 fuzzy sets and multiplicative half quadratic programming-based MCDM framework for calculating aggregated risk ranking results of failure modes in FMECA*. Pages 194-222.

Failure modes, effects and criticality analysis (FMECA) is a popular methodology among the safety, reliability, and risk engineers, which can identify the potential failure modes of a system, process, or design, evaluate their cause(s), and rank them according to their criticality. The traditional risk priority number (RPN)-based risk ranking approach has multiple limitations, and researchers have been employing multi-criteria decision making (MCDM) methods to address those drawbacks. In this work, a novel integrated framework is proposed with threefold contributions. Firstly, to minimize the associated linguistic uncertainties during the evaluations of failure modes with respect to the risk factors, the concept of interval type-2 fuzzy sets (IT2FSs) is used. Secondly, to portray the causal dependencies among the risk factors and to compute their weights, an extended IT2F-DEMATEL (Decision Making Trial and Evaluation Laboratory) method is proposed for the group decision-making scenario. Thirdly, the risk ranking results of failure modes are calculated by proposing the concepts of IT2F-MAIRCA (Multi-Attributive Ideal Real Comparative Analysis), IT2F-MARCOS (Measurement of Alternatives and Ranking according to COmpromise Solution) methods, and modified IT2F-TOPSIS (Technique for Order of Preference by Similarity to Ideal Solution) methods. Further, after observing that each of the proposed method calculates different ranking results of failure modes, the concept of half-quadratic (HQ) minimization is used to calculate the aggregated ranking results along with the consensus index and trust level. The potential

of the integrated framework is highlighted by considering a benchmark FMECA example of a process plant gearbox. Finally, sensitivity analyses are carried out to observe the robustness of the proposed framework, and each of the developed method.

- **Keywords:** FMECA; Extended IT2F-DEMATEL; IT2F-MAIRCA; IT2F-MARCOS; Half-quadratic minimization; MCDM

Jiacheng Sun, Chengyuan Su, Ying Xie, Zhi Huang, Jiayi Bao, Menglin Chen, Xiangfeng Lin. *Rare earth mine wastewater treatment via modified constructed rapid infiltration system: Nitrogen removal performance and microbial community*. Pages 223-232.

The treatment of ion-type rare earth mine (REM) wastewater by a modified constructed rapid infiltration system (CRIS) was explored. Meanwhile, the activities of hydroxylamine oxidase, nitrite reductase and urease in the column were measured, and the microorganisms in the system were analyzed. When the hydraulic load was 0.1 m3 m−2·d-1, the column height had a significant influence on the NH4+-N and TN removal rates. Specifically, the average NH4+-N and TN removal rates were 29.06 % and 14.83 %, respectively, for the CRIS with a 100 cm single-layer inorganic filler layer. While the average NH4+-N and TN removal rates increased to 69.70 % and 38.90 %, respectively, for the CRIS with a 140 cm double-layer inorganic filler layer. After increasing the hydraulic load from 0.1 m3 m−2·d-1 to 0.2 m3 m−2·d-1, the average NH4+-N and TN removal rates increased by 29.61 % and 15.84 %, respectively, in the long CRIS. The activities of hydroxylamine oxidase, nitrite reductase and urease in the column also improved. Nitrite reductase increased to 0.605 nitrite/min mg protein and hydroxylamine oxidase increased to 0.470 U/ mL g in the lower layer of the long CRIS. High-throughput sequencing analysis showed that the dominant bacterial phyla was mainly Proteobacteria and Planctomycetes. Pseudomonas, Bacillus and other aerobic denitrifying bacteria were detected at the genus level, as were the anaerobic denitrifying bacteria Comamonas and Thauera. These results illustrated that aerobic denitrification, anaerobic denitrification and anaerobic ammoxidation simultaneously existed during the CRIS treatment of REM wastewater to achieve TN removal. Furthermore, when using two full-scale CRIS in a series to treat actual REM wastewater, the NH4+-N removal rate reached 99.14 %.

- **Keywords:** Modified constructed rapid infiltration systems; Rare earth mine wastewater; Hydraulic load; Aerobic denitrification; Microbial community

Liuyang Ma, Qin Zhao, Xinru Guo, Houcheng Zhang, Ziyang Hu, Shujin Hou. *A hybrid system consisting of dye-sensitized solar cell and absorption heat transformer for electricity production and heat upgrading*. Pages 233-241.

A new hybrid system mainly composed of a dye-sensitized solar cell (DSSC), a solar selective absorber (SSA) and an absorption heat transformer (AHT) is theoretically put forward to harness the long wavelength sunlight transmitted through the DSSC. The models of both DSSC and AHT are adopted from the current literature and the condition enables the AHT to involve in heat upgrading is obtained. The model validations of DSSC and AHT are conducted using experimental data. Mathematical expressions of power output and efficiency for the hybrid system are formulated by taking a variety of irreversible losses into account. The effectiveness of the hybrid system is justified and evaluated. Maximum power density (MPD) and maximum energy efficiency (MEE) of the integrated system are, respectively, 158.2 W m−2 and 16.3 %, having evidently improvement compared to that of a single DSSC. A variety of operating conditions and design parameters affecting the hybrid system performance are studied. Numerical calculation results show that the working temperature, photoelectron absorption coefficient of DSSC and total heat-transfer area of the AHT have positive effects on the

hybrid system performance. There exists an optimum TiO2 thin film thickness to optimize the hybrid system performance. However, a greater Schottky barrier has negative influence on the hybrid system performance. The results obtained here may provide some guidance for designing such a practical hybrid system.

- **Keywords:** Dye-sensitized solar cell; Absorption heat transformer; Efficiency; Power output; Sensitivity analysis

Cong Jing, Jiaxing Zhu, Leping Dang, Hongyuan Wei. *Simultaneous design for a complex heterogeneous wastewater separation and recovery process: process improvement, plantwide control and safety analysis*. Pages 242-258.

Recently, a new industrial relevant wastewater (water/Cyclohexane/sec-butyl alcohol) separation process with vapor recompression and thermal coupling was proposed as the conventional homogeneous extractive distillation. This highly integrated and interactive multivariable process presents great challenges to the dynamic controllability and process safety analysis. In this paper, based on the concept of "simultaneous design", the newly proposed process is systematically investigated from the perspective of process improvement, plantwide control and safety analysis. Firstly, for energy conservation and CO2 emission reduction, the new complex process is further improved by applying the features of heterogeneous distillation. And a modified heterogeneous distillation process with heat pump is proposed, which can save reboiler duty about 16.8 % and save compressor electricity up to 67.7 %, while the reduction of CO2 emissions is 23.5 %. Secondly, for the efficient heterogeneous distillation process, an effective and robust plantwide control strategy is developed and tested under large throughput and feed composition disturbances. Last, with the dynamic simulation assisted HAZOP, a quantitative safety analysis is conducted, which can help experts to consider the nature, scale and response time of hazards and identify the potential propagation of deviation between different units, and then propose more specific or accurate safety recommendations correspondingly.

- **Keywords:** Wastewater treatment; Heterogeneous distillation; Controllability; Safety analysis; HAZOP

Kening Li, Ronghui Zhang, Haiwei Wang, Fan Yu. *Multi-intelligent connected vehicle longitudinal collision avoidance control and exhaust emission evaluation based on parallel theory*. Pages 259-268.

With the increasing of vehicle volume and driving speed, traffic accidents and environmental safety have become social concerns. Vehicle traffic accidents, especially multi-vehicle chain accidents, cause damage to property and human lives. Meanwhile, traffic pollution will lead to continuous harm to living environment and health. This is a coupled human-vehicle-environment interaction system, which is difficult to model with traditional mathematical methods. Parallel theory is an effective method to solve such complex problems based on advanced artificial intelligence and computer technology. In this paper, a parallel system is built to analyze and control multi-intelligent connected vehicle based on parallel theory. The parallel system is also used to analyze and assess the exhaust emission of multi-intelligent connected vehicle. The parallel system is carried out with three steps: 1) modeling and representation of multi-intelligent connected vehicle system using artificial societies; 2) analysis and evaluation by computational experiments; 3) control, management and exhaust emission evaluation through parallel execution of real and artificial systems and big data. The parallel control methods, models and conclusions obtained from this paper can be used to enhance the experience of safety in multi-vehicle control under vehicle to everything environment and make the safety intervention measures more efficient.

- **Keywords:** Traffic accidents; Collision avoidance control; Exhaust emission evaluation; Parallel theory; Safety intervention

Ping Liu, Lukuan Yang, Li Sun. *Multi-objective economic model predictive control of wet limestone flue gas desulfurisation system*. Pages 269-280.

Control of wet limestone flue gas desulfurisation (WFGD) system is critical for pollution reduction of the coal-fired power plant. To fulfill the environmental requirements with the least cost, economic model predictive control (EMPC) is utilized in this paper to tackle the difficulties of WFGD, such as nonlinearity, couplings and trade-off between efficiency and safety. First, a comprehensive first-principle model is developed to describe the overall nonlinear characteristics of WFGD, with special considerations on Gas-to-liquid contact zone and slurry pool module. Second, four objectives are formulated to evaluate the economic criterion from different perspectives, including cost, safety, control efforts and performance. Utopia strategy, combined with NSGA-II, is used to solve the EMPC problem and obtain the Pareto front of the multi-objective optimization. Simulation results show that the proposed strategy is able to efficiently ensure the emission requirement and reduce the economic cost simultaneously, regardless of load disturbance, adjustment of emission lower limit and fluctuation of limestone market price.

- **Keywords:** First-principle modelling; WFGD; Economic model predictive control; Multi-objective optimization

Yu Jianxing, Wu Shibo, Yu Yang, Chen Haicheng, Fan Haizhao, Liu Jiahao, Ge Shenwei. *Process system failure evaluation method based on a Noisy-OR gate intuitionistic fuzzy Bayesian network in an uncertain environment*. Pages 281-297.

In the system reliability evaluation of the process industries, it is sometimes difficult to get precise and sufficient failure data of system components utilized to calculate the failure probability. In this study, a Noisy-OR gate Bayesian network method based on intuitionistic fuzzy theory is proposed in cases of imprecise and insufficient historical data. The main contributes of this method include: a set of triangular intuitionistic fuzzy numbers considering uncertainty and hesitation is defined based on the standards and industry practices, meanwhile, a corresponding probability conversion method is also proposed; an improved similarity aggregation method is employed for less uncertainty accumulation and reducing the deviation caused by individual differences during the aggregation; the uncertain causal relationship among the relevant nodes is determined by applying the Noisy-OR gate in the Bayesian network. Furthermore, a case study of the crude oil tank fire and explosion accident is performed to illustrate the applicability of proposed approach. The comparison between the obtained results and that from pre-existing methods shows that the proposed method can provide a more suitable result in an uncertain environment. The weak links of the crude oil tank system are identified through Bayesian reasoning and sensitivity analysis, which can aid decision-making and improve the security execution of the crude oil tank system.

- **Keywords:** Failure evaluation; Uncertainty; Bayesian network; Intuitionistic fuzzy number; Noisy-OR gate model; Crude oil tank fire and explosion

Umakant Badeti, Niren Kumar Pathak, Federico Volpin, Ugyen Dorji, Stefano Freguia, Ho Kyong Shon, Sherub Phuntsho. *Impact of source-separation of urine on effluent quality, energy consumption and greenhouse gas emissions of a decentralized wastewater treatment plant*. Pages 298-304.

The impact of urine diversion on the biological treatment processes at a decentralized wastewater treatment plant (WWTP) was investigated. BioWin software was used for the simulations, and the model was firstly validated with data from a real WWTP. The simulations showed that upto 82 % N, 30 % P, 6% chemical oxygen demand (COD) load to the WWTP can be reduced by complete urine diversion but effluent N reduction was notable up to 75 % urine diversion. Under the current WWTP operating conditions, the simulations suggest that 33 % of aeration energy can be saved by 90 % urine diversion. Direct N2O and CO2 emissions in the treatment processes can also be reduced by 98 % and 25 % respectively. Indirect green house gas emissions can also be reduced by 20 %. Overall, the reduction in the discharge of nutrients and in the operation of blowers was found to contribute to a 22 % reduction in the operating costs (on energy consumption and nutrient discharge).

- **Keywords:** Source separation of urine; Nitrogen removal; Environmental impacts; Greenhouse gas emissions

Chuyuan Huang, Xianfeng Chen, Lijuan Liu, Hongming Zhang, Bihe Yuan, Yi Li. *The influence of opening shape of obstacles on explosion characteristics of premixed methane-air with concentration gradients*. Pages 305-313.

By installing obstacle plates with different opening shapes in an experimental pipeline, the combined effect of vertical concentration gradients and obstacle shapes on methane-air explosion characteristics was experimentally investigated. The presence of obstacles and concentration gradients induced turbulent flame instabilities, which promoted the positive feedback between the combustible gas flow and combustion process. The combustion process caused the upstream lean methane, lighter than the unburned gas, to propagate through the obstacle and hence bubble-like local disturbances were generated in the central area downstream of the obstacle. Under the action of transverse waves, a "gap" appeared in the lower part of the flame front, and the flame front appeared concave. The effect of the concentration gradient and obstacles on the methane explosion gradually weakened, and hence the wrinkled flame surface gradually stabilized. Results show that the square-shaped opening affected the flame propagation and explosion evolution most significantly. As the concentration gradient increased, the combined effect undermined the positive feedback mechanism, and the maximum explosion overpressure and maximum rate of pressure rise were reached for the square-shaped opening at a low concentration gradient (0.5 %), while for the circular-shaped and quadrant-shaped openings the maximum values were reached at a higher concentration gradient (1.0 %). The effect of obstacles was more significant than the effect of concentration gradients with respect to the flame propagation velocity and rate of pressure rise.

- **Keywords:** Concentration gradient; Opening shape; Obstacle plate; Methane-air; Explosion characteristics

Abhinesh Kumar Prajapati. *Sono-assisted electrocoagulation treatment of rice grain based distillery biodigester effluent: Performance and cost analysis*. Pages 314-322.

Electrocoagulation process coupled with sonication is a type of advance oxidation process (AOP) to treat different type of waste waters. Biodigester effluent (BDE) generated from distillery industry contains very high chemical oxygen demand (COD=5500 mg/dm3) with high color (510 PCU) appearance. Organics reduction of biodigester effluent (BDE) in term of chemical oxygen demand (COD) and color have been investigated in a batch sono-electrocoagulation reactor with different electrode combinations such as Fe-Fe, Al-Al, Fe-Al, and Al-Fe at ultrasound frequency of 40 kHz. The impact of different operating

parameters such as electrolyte concentration, electrode combination, pH and current density (CD) on COD and color removal are evaluated. The electrode combination of Fe-Fe has provided better results in sono-electrocoagulation process as compared to sonication and electrocoagulation alone. The maximum COD and color reduction efficiency of 99.1 % and 61.6 % was found at the electrode combination of Fe/Fe, CD 69.44 A/m2, pH 8, NaCl concentration 5 mg/dm3, and process time of 125 min. On the other hand the maximum COD and color removal efficiency of 98.3 % and 58.1 % was observed with the electrode combination of Al-Al at same operating conditions as described for Fe. Finally, sludge analysis and cost optimization are also incorporated in this article. It is found that at optimum condition (electrode combination of Fe/Fe, CD 69.44 A/m2, pH 8, NaCl concentration 5 mg/dm3, and process time of 125 min) the operating cost of the process is 1.39 $/m3. Sludge obtained after the treatment process contains anodic material (0.07 kg iron for the treatment 1 m3 of BDE) and also sludge had good heating value (5.5 MJ/kg). This work demonstrated that sono-electrocoagulation process is well applicable to treat BDE.

- **Keywords:** Biodigester effluent; Sono-electrocoagulation; Iron electrode; Aluminium electrode; Power consumption

Samyuktha S. Kolluru, Shreya Agarwal, Sadamanti Sireesha, I. Sreedhar, Samir Ramdas Kale. *Heavy metal removal from wastewater using nanomaterials-process and engineering aspects*. Pages 323-355.

Nanomaterial adsorbents are highly favorable for heavy metal removal due to their large specific surface areas with enhanced active sites for contaminant adsorption. This paper focuses on nanomaterial adsorbents covering aspects like methods of synthesis, types of nanomaterials, kinetics, process optimization, modelling and simulation and column studies besides citing future challenges. It has been found that among various synthesis protocols, Chemical Vapor Deposition was most effective in giving desired attributes. Metallic composites and organic nanomaterials viz. nanocellulose, carbon nanotubes, graphene complexes, magnetite forms etc exhibited highest metal removal capacities of 1989 mg/g for Hg (II) 1641 mg/g for Cd (II) at optimal process conditions. Eco-friendly nanomaterial adsorbents, their properties and potential are also discussed in detail. This work also explores the performance of nanomaterials in fixed bed columns where it showed its capability to be used as an effective adsorbent in continuous adsorption mode.

- **Keywords:** Nanomaterials; Heavy metal adsorption; Synthesis protocols; Eco-friendly; Regeneration; Dynamic adsorption; Optimization; Simulation; Fixed bed columns

Lau N. Jun, Mahadi B. Bahari, H.D. Setiabudi, A.A. Jalil, Dai-Viet N. Vo. *Greenhouse gas mitigation and hydrogen generation via enhanced ethylene glycol dry reforming on La-promoted Co/Al2O3 catalyst*. Pages 356-364.

The first investigation of La-promoted Co/Al2O3 catalysts in Ethylene Glycol-CO2 conversion (EGCC) for syngas (H2 + CO) production was conducted in this work. Co/Al2O3 catalysts modified with different La promoter loadings (1, 3, and 5%) were generated through sequential incipient wetness impregnation technique and employed for EGCC. The physicochemical attributes of the generated catalysts were examined via Brunauer-Emmett-Teller (BET), H2 temperature-programmed reduction (H2-TPR), X-ray diffraction (XRD), Raman, and temperature-programmed oxidation (TPO). 3%La-promoted catalyst owned the largest specific surface area, smallest Co crystallite size of 9.8 nm, and lowest reduction temperature among the promoted catalysts. These excellent properties resulted in the highest catalytic performance on the 3%La-promoted

catalyst (i.e., C2H6O2 conversion = 77.6 %, CO2 conversion = 43.1 %, H2 yield = 75.3 %, and CO yield = 76.8 %). The significant reduction in carbon deposition of the 3%La-promoted catalyst was due to the La capability in eliminating deposited carbon via the formation of intermediate lanthanum dioxycarbonate, La2O2CO3.

- **Keywords:** Ethylene glycol; Cobalt; Syngas; La promoter; CO2 conversion; Hydrogen

Ali Ansari, Enrico Tapire Nadres, Minh Đỗ, Debora Frigi Rodrigues. *Investigation of the removal and recovery of nitrate by an amine-enriched composite under different fixed-bed column conditions*. Pages 365-372.

Continuous adsorption of nitrate in a fixed-bed column can be an effective method for its removal from water. In this study, an amine-rich polymer composite adsorbent was prepared by crosslinking chitosan (CS) and polyethyleneimine (PEI) with glutaraldehyde (GLA). The CS-PEI-GLA was packed into columns and the effect of flow rate, influent concentration, bed height, and other ionic species on the column performance was investigated. The highest adsorption capacity was achieved at the lowest flow rate and highest influent concentration and bed height. Maximum adsorption capacity of 137.62 mg NO3−-N/g was determined from the Thomas model. The column had acceptable nitrate removal in the presence of 1000 ppm chloride but poor performance in the presence of 1000 ppm sulfate due to the competitive effect of sulfate for binding sites. The best recovery agent was 0.5 M NaCl as it could regenerate the column to <90 % of its capacity after 10 adsorption-desorption cycles. The adsorbent effectively removed nitrate as well as phosphate and total organic carbon from a real water sample. This study suggests that amine rich polymers can be good candidates for the removal of nitrate in contaminated water.

- **Keywords:** Nitrate; Chitosan; Polyethyleneimine; Continuous adsorption; Breakthrough models

Kazuko Yui, Hidetoshi Kuramochi, Masahiro Osako. *Measurement and modeling of heavy metal behaviors during the incineration of RDF in a pilot-scale kiln incinerator-Part 1: Modeling using multizonal thermodynamic equilibrium calculation*. Pages 373-384.

Multizonal thermodynamic equilibrium calculation is one of the methods used in estimating or explaining the fate of elements such as heavy metals during waste incinerations and probably only one method that can estimate the fate of trace elements, but the ability of the calculation as a fate-estimation tool was not fully examined. This study examines the performance of multizonal thermodynamic equilibrium calculation applied to waste incineration by comparing the calculated results with the results from the incineration test and literature information. High temperature behaviors of the heavy metals were also reviewed to correctly understand their gas phase speciation in the incinerator, and the thermodynamic data of gaseous Cd species were modified to better reproduce the high temperature vaporization behavior. The calculation represented the high volatility of Hg, Cd, Pb, and low volatility of Cr in the incineration, whereas the measured high volatility of Zn and As could not be obtained by the calculation. The calculation succeeded in reproducing the possible gas phase chemical speciation of heavy metals in the incinerator expected from the review on the high temperature properties, whereas the calculated fly ash speciation does not match with the measured speciation. Possible reasons for these inconsistencies were considered.

- **Keywords:** Thermodynamic equilibrium calculation; RDF; Municipal solid waste; Incineration; Heavy metal

Giordano Emrys Scarponi, Gabriele Landucci, Albrecht Michael Birk, Valerio Cozzani. *Three dimensional CFD simulation of LPG tanks exposed to partially engulfing pool fires*. Pages 385-399.

The availability of accurate and robust models for the prediction of the behavior of pressurized tanks under fire exposure is a key requirement to improve the design of fire protection systems. Most of the models present in the literature take into consideration fully engulfing pool fire scenarios only. In the present study, a CFD modelling approach previously validated against full engulfing pool fire tests is used to simulate partial engulfment conditions. The model allowed analyzing local flow field promoting thermal stratification, which in turn drives internal pressurization of the tank. Comparison with fire test results shows good agreement with experimental measurements both in terms of temperature and pressurization curves. The results obtained represent a valuable source of information to support risk management, planning of emergency response and improve fire protection systems design.

- **Keywords:** LPG tank; Partial engulfment; Pressure vessel exposed to fire; Thermal stratification; CFD modeling

Jun Lu, Changbao Jiang, Zhuo Jin, Wensong Wang, Wanjun Zhuang, Huan Yu. *Three-dimensional physical model experiment of mining-induced deformation and failure characteristics of roof and floor in deep underground coal seams*. Pages 400-415.

Underground mining engineering causes complex changes in the three-dimensional stress near the working face of a mine, resulting in deformation and failure of the roof and floor rocks, as well as ground subsidence. To study the stress, deformation, and fracture field characteristics of the roof and floor strata due to mining, an indoor large-scale three-dimensional physical similarity model was developed. A novel method was used to simulate the mining process of coal seams. The results show that coal seam mining disrupted the original stress balance; consequently, a bearing pressure was generated in front of the working face, and a significant pressure relief state appeared in a particular area. The collapsed rock blocks of the overburden strata filled the goaf and played a supporting role, causing the overburden stress to increases again to a value close to the original rock stress. After complete mining, the overburden strata subsided, and the floor strata bulged. With an increasing vertical distance from the working face, the deformation of the rock formation gradually decreased. Evident fractured fields were formed in the surrounding rock of the goaf. In the horizontal section of the overburden rock layer, the cracks were distributed in a "rounded rectangular" shape. As the distance from the coal seam increased, the "rounded rectangular" boundary became smoother; the coverage area decreased; and the degree of crack opening and development in the plane decreased. The fractal dimensions of fractures with different overburden heights and different strike positions are calculated using the fractal geometry theory. We found that as the distance from the excavation face increased, the fractal dimensions of the fractures gradually became stable. In addition, numerical simulation methods were used to verify the correctness of the physical similarity model experiments. The research results can provide important references for the stability of deep underground projects such as coal mining process, tunnel excavation process, nuclear waste storage and other engineering stability.

- **Keywords:** Three-dimensional physical similarity model; Deep coal mines; Mining-induced stress; Fracture field; Numerical simulation

Md Alauddin, Faisal Khan, Syed Imtiaz, Salim Ahmed, Paul Amyotte. *Pandemic risk management using engineering safety principles*. Pages 416-432.

The containment of infectious diseases is challenging due to complex transmutation in the biological system, intricate global interactions, intense mobility, and multiple transmission modes. An emergent disease has the potential to turn into a pandemic impacting millions of people with loss of life, mental health, and severe economic impairment. Multifarious approaches to risk management have been explored for combating an epidemic spread. This work presents the implementation of engineering safety principles to pandemic risk management. We have assessed the pandemic risk using Paté-Cornell's six levels of uncertainty. The susceptible, exposed, infected, quarantined, recovered, deceased (SEIQRD), an advanced mechanistic model, along with the Monte Carlo simulation, has been used to estimate the fatality risk. The risk minimization strategies have been categorized into hierarchical safety measures. We have developed an event tree model of pandemic risk management for distinct risk-reducing strategies realized due to natural evolution, government interventions, societal responses, and individual practices. The roles of distinct interventions have also been investigated for an infected individual's survivability with the existing healthcare facilities. We have studied the Corona Virus Disease of 2019 (COVID-19) for pandemic risk management using the proposed framework. The results highlight effectiveness of the proposed strategies in containing a pandemic.

- **Keywords:** Risk analysis; Pandemic; Non-pharmaceutical interventions; Precautionary principle; ALARP; COVID-19

Lichao Lu, Zenab Tariq Baig, Dong Dong, Jinying Xi. *Preparation and characterization of a novel packing material for the gas-phase fluidized-bed bioreactor*. Pages 433-439.

Gas-phase fluidized-beds reactor (FBR) can overcome the shortages of bed clogging and performance decline in packed-bed reactors on VOCs treatment. Ideal FBR packing materials with minimum fluidized velocity and surface characteristics are required. In this study, an expanded polystyrene (EPS) with particle size 1.0–2.0 mm was selected as the skeleton among six types of EPS and two types of expanded polypropylene (EPP). They were then physically coated with a combination of potato dextrose medium, fine wheat bran particles, and inorganic glue. Different glue concentrations and amounts of medium were tested and the optimal values of 2 % and 0.22 g·cm−2 were achieved. The wheat-coated EPS obtained hydrophilic functional groups on the surface, and its contact angle decreased from 93° to 37° after coating. By scanning electronic microscopy, more microorganisms were observed on the surface of the coated EPS than that of the uncoated EPS. A lab-scale fluidized bioreactor was built to treat gaseous ethanol. The minimum fluidized velocity of coated packing materials was 0.2 m·s−1 under a relative humidity of 50 ± 10 %, reaching an average elimination capacity of 681 g m-3 h−1 during the 28-days operation, while the bioreactor packed with uncoated EPS reached only 18 g m−3 h−1.

- **Keywords:** Gaseous VOC purification; Fluidized bed bioreactor; Packing material

M.M. Younes, A.S. Abdullah, F.A. Essa, Z.M. Omara, M.I. Amro. *Enhancing the wick solar still performance using half barrel and corrugated absorbers.* Pages 440-452.

The performance of tilted wick solar stills including new absorber configurations have been investigated. Four solar stills are built, the first one is flat wick solar still (FWSS), the second one is corrugated wick solar still (CWSS), the third one is half barrel wick solar still (BWSS) and the fourth one is conventional solar still (CSS). The modification in the absorber configuration increases the evaporation area for CWSS and BWSS. The new absorber designs are used to reduce the water flow rate through wick to improve the evaporation rate. The measurements showed that, the increase in the daily yields when compared with CSS are 75 %, 93 % and 100 % for FWSS, BWSS and CWSS,

respectively. The theoretical model shows acceptable agreement with the measured data. For further enhancement in wick solar still performance, BWSS and CWSS have been tested with phase change material (PCM) mixed with CuO nanoparticles. The results obtained that, the daily productivity for CWSS and BWSS is increased to be 134 % and 124 % over CSS, respectively. Also, the efficiency and calculated cost per liter are 35 %– 0.028 $, and 54.5 % –0.023 $ for CSS and CWSS with phase change material, respectively.

- **Keywords:** Solar still; Wick; Corrugated absorber; Half barrel; Thermal storage material; Nanoparticles

Zhongyang Zhao, Yongxin Zhang, Wenchao Gao, Jakov Baleta, Chang Liu, Wenjun Li, Weiguo Weng, Haobo Dai, Chenghang Zheng, Xiang Gao. *Simulation of SO2 absorption and performance enhancement of wet flue gas desulfurization system*. Pages 453-463.

At the present moment wet flue gas desulfurization systems (WFGD) are widely used in the SO2 emitting industries. With the improvement of the SO2 emission standards and the use of fuel with high sulfur content, there is an urgent need to develop advanced modelling tools to explore the enhancing method of SO2 absorption process on the condition of flue gas with high SO2 concentration. In this study, a detailed mathematical model of tray scrubbers, which are adopted in several China's power plants in order to treat SO2 rich flue gas, is developed to investigate the influencing factors of the SO2 absorption process. The model is validated by an experiment using pilot-scale WFGD experimental system and can describe the SO2 absorption process in WFGD to a satisfactory level. The influence factors of SO2 absorption of droplets and in spray tower are studied through the model. The effects of pH and tray on desulfurization efficiency are analyzed. Using the tray scrubber is better in order to realize the desulfurization of flue gas with high SO2 concentration rather than adjusting the pH of the slurry. This model can be regarded as a useful tool for equipment selection and operation optimization of WFGD system.

- **Keywords:** SO2 absorption; Tray scrubber; High SO2 concentration; Performance enhancement

Mengxi Yu, Madhav Erraguntla, Noor Quddus, Costas Kravaris. *A data-driven approach of quantifying function couplings and identifying paths towards emerging hazards in complex systems*. Pages 464-477.

Hazardous scenarios emerging from complex system where number of functions are large and corresponding function coupling are humongous, are very difficult if not impossible to identify humanly. Today's complex systems generate a very large dataset every minute and dynamic nature of the generated data makes it difficult to track such couplings. The Functional Resonance Analysis Method (FRAM) got success in recent years to understand hazards emerging from function couplings in complex systems, however, challenges remain to estimate aggregated couplings appropriately without quantitative analysis. The current study developed a data-driven approach to quantify function couplings using lift confidence intervals of association rules. Later, association rules were merged to identify the paths leading to a potential hazardous scenario. The paths were presented graphically and equipped with quantified coupling information and capable of providing guidance to prevent the emerging hazard scenario. The approach has been demonstrated with a case study of a polymerization process in process industry for which function couplings are represented by a very large dataset.

- **Keywords:** Complex system; FRAM; Association rule mining; Hazard identification; Bootstrap

Aitao Zhou, Meng Zhang, Kai Wang, Derek Elsworth, Nan Deng, Jiaying Hu. *Rapid gas desorption and its impact on gas-coal outbursts as two-phase flows*. Pages 478-488.

Coal and gas outbursts are a violent release of energy in part driven by rapidly desorbing gas from the fragmenting coal. We present a coupled two-phase model of coal and gas outbursts to define the timing, rate and magnitude of gas desorption and its contribution to the resulting energetics. The model involves a fragmenting ejection of the outburst from an overpressurized coal that retreats omnidirectionally from a point and develops a deepening crater. This model is applied to represents both experiments and in situ observations. These results indicate that the outburst is initially driven by free gas before desorbing gas rate exceeds this free gas liberation rate early into the outburst (at ~17 s in our model). The cumulative mass of desorbed gas only exceeds the free gas later into the event at approximately double this duration (at ~29 s in our model). During the outburst, ~55 % of the expansion energy is contributed by desorbing gas. Using the initial gas emission rates for both non-tectonic and tectonic coals defines a power-law relationship between the initial gas desorption rate and the desorption gas contribution (~14 %–92 %), indicating that the desorbing gas plays a decisive role in outburst development. Furthermore, taking the gas emission model as a boundary conditions for numerical simulations, the gas pressure potential energy (GPPE) released in the first millisecond at the maximum gas emission rate is derived to characterize its effects on the dynamic characteristics of the outburst two-phase flow. The maximum energy release intensity considering gas desorption is ~5 times that without gas desorption for non-tectonic coal. For tectonic (mylonitized) coals the energy release is a further ~4 times greater than that of non-tectonic coals. This paper presents a novel quantitative study defining the role of gas desorption in outbursts and contributes to the understanding of causal mechanisms and precursory phenomena preceding catastrophic outbursts.

- **Keywords:** Coal and gas outburst; Gas emission model; Contribution of desorption gas; Quantitative study; Outburst two-phase flow

Zizhao Chen, Dirui Wu, Liang Chen, Mengxin Ji, Jun Zhang, Yuying Du, Zhengshun Wu. *The fast co-pyrolysis study of PVC and biomass for disposing of solid wastes and resource utilization in N2 and CO2*. Pages 489-496.

This study investigated the fast pyrolysis of polyvinyl chloride (PVC) and wood powder (WP). Thermogravimetric analyzer (TGA) was used to study their pyrolysis characteristics in N2 and CO2, and the interaction of them were studied in a fixed bed reactor. The results showed that the addition of WP advanced the two stages of the pyrolysis of PVC and increased the maximum weight loss temperature, the pyrolysis modes of PVC and WP were same in N2 and CO2. Monocyclic aromatic hydrocarbons increased after WP was added, while the aromatic hydrocarbons with more than six carbons decreased. And the more WP was added, the more obvious the inhibitory effect. Compared with pyrolysis in N2, CO2 improve further the pyrolysis efficiency of waste and effectively inhibited the generation of harmful substances such as PAHs. The content of CO and CO2 increased and the content of CH4 and H2 decreased when WP was added. According to the experimental results, the mechanism of formation of the monocyclic aromatic hydrocarbon was deduced. These studies provided a theoretical basis for the co-pyrolysis of PVC and biomass to obtain low carbon hydrocarbons.

- **Keywords:** Polyvinyl chloride (PVC); Wood powder (WP); Pyrolysis; Polycyclic aromatic hydrocarbons (PAHS); Carbon dioxide

Jandira Leichtweis, Siara Silvestri, Nicoly Welter, Yasmin Vieira, Paloma I. Zaragoza-Sánchez, Alma C. Chávez-Mejía, Elvis Carissimi. *Wastewater*

***containing emerging contaminants treated by residues from the brewing industry based on biochar as a new CuFe2O4 / biochar photocatalyst*. Pages 497-509.**

A novel green composite catalyst was prepared by doping CuFe2O4 nanoparticles in the malt bagasse biochar. Composites with different ratios of malt biochar and CuFe2O4 were produced and characterized by XRD, FE-SEM, EDS, HR-TEM, UV–vis, and Zeta potential. The results revealed that CuFe2O4 was successfully supported on the malt biochar surface. The prepared composites showed the band gap energies were narrower than of CuFe2O4, increasing the photocatalytic activity. At 60 min of heterogeneous photo-Fenton, tests under visible light indicated CuFe2O4 removed 39 % of the rhodamine B color, while composites CFO1B3, CFO1B1, and CFO3B1 removed 88 %, 81 %, and 44 % of the dye, respectively. The recycling of the CFO1B3 composite indicated that it can be used in eight cycles without major losses in efficiency. In sunlight, the CFO1B3 composite achieved efficiencies of 100 % for 10 mg L−1 and 50 mg L−1 of rhodamine B at 10 and 20 min of reaction, respectively. In the proposed mechanism, it was verified that the radical OH, O2− and h+ were the predominant reactive species involved in the degradation to intermediates of low m/z. Results showed that the novel composite formed is a promising photocatalyst for removing organic pollutants in water.

- **Keywords:** Malt biochar; CuFe2O4/biochar; Visible light photo-Fenton; Solar photo-Fenton

Jianqin Zheng, Jian Du, Yongtu Liang, Qi Liao, Zhengbing Li, Haoran Zhang, Yi Wu. *Deeppipe: A semi-supervised learning for operating condition recognition of multi-product pipelines*. Pages 510-521.

Intelligent operating monitoring of pipelines helps to detect anomalies in time to ensure pipeline safe, reducing potential risk. However, the operating conditions of the multi-product pipeline change frequently, and the recognition and monitoring by on-site personnel are easy to cause misjudgment, so the operating conditions of the pipeline cannot be accurately recognized. Noticeably, operating condition recognition is an important part of pipeline safety and risk management. Although ample operating data are stored in SCADA system, these data are lack of corresponding condition labels, making it hard to be mined. In this work, a semi-supervised learning for operating condition recognition is proposed to overcome aforementioned issues. Firstly, the operating parameters of each station are preprocessed and collected to construct into data matrices to overcome transient disturbance considering the pipeline space characteristics and time series of the operating data. Then stacked autoencoder (SAE) is used to pre-train the network parameters of multi-layer neural network (MLNN) based on a large amount of unlabeled operating data. After that, MLNN is fine-tuned based on a small amount of labeled data annotated by referring to the operation log. To verify the effectiveness of the semi-supervised learning, a real multi-product pipeline is taken as an example for operating condition recognition. The accuracy, precision, recall and F1 score is 95 %, 95 %, 80 % and 80 %, respectively. Results show that the condition recognition accuracy of the proposed model is better than other machine learning models. Finally, the sensitivity analysis is conducted to illustrate the importance of SAE in this classification model.

- **Keywords:** Pipeline; Operating condition recognition; Semi-supervised learning; Sensitivity analysis

Jianfeng Zhou, Genserik Reniers. *Area impact analysis of chemical installations and critical installations identification*. Pages 522-531.

Identifying critical installations in an area containing many chemical installations is important for the safety management of the chemical area. In this study, the area impact degree of chemical installations is defined, which is determined by analyzing the probability of accidents at other installations in the area when an accident occurs at a given installation, and the losses caused by each installation in the event of corresponding accident. Critical installations for area safety can be easily identified by comparing the area impact degree of different installations in the area. An illustrative example demonstrates the proposed approach. Analysis of the area impact degree of 6 tanks in a storage area and identification of more important installations for the safety of the entire area illustrate the applicability of this approach. Furthermore, our novel area importance analyzing approach is also compared with the graph approach.

- **Keywords:** Chemical area; Critical installation; Area impact degree; Domino effect

Omar Fawzi Suleiman Khasawneh, Puganeshwary Palaniandy. *Occurrence and removal of pharmaceuticals in wastewater treatment plants*. Pages 532-556.

Pharmaceutical compounds, such as antibiotics, nonsteroidal anti-inflammatory drugs (NSAIDs), anticonvulsants, β-blocker, etc. have emerged as new classes of water pollutants due to their potential or proven adverse effects on human health and the aquatic environment. This paper aims to systematically review the current data available on the global occurrence and removal of 43 pharmaceutical compounds in municipal wastewater treatment plants (M-WWTPs) in the period from 2010 to 2020. Moreover, this work intends to assess the global daily mass load and emissions of pharmaceuticals in different regions. Nevertheless, the environmental risk of pharmaceuticals in the final effluents of M-WWTPs was also evaluated. Lastly, the guidelines and regulations concerning the occurrence of pharmaceuticals in the aquatic environment were summarized and discussed. The findings highlighted that there is significant variation in the concentrations of pharmaceuticals between different regions. Meanwhile, the concentrations of pharmaceuticals in the influents of Asian region tend to be higher than those in other monitored regions. In this respect, the highest average daily mass loads were observed for acetaminophen (473 g/1000 in./day) and atenolol (592 g/1000 in./day), while amoxicillin (944 g/day), sulfamethoxazole (688.38 g/day) recorded the highest daily emissions. The environmental risk assessment based on the risk quotient (RQ) showed that twelve of the monitored pharmaceuticals pose a high potential risk to the aquatic ecosystems. The emphasized guidelines and regulations laid focus on the measures that can be used to mitigate the occurrence of pharmaceuticals in the environment. Research needs and future recommendations are also identified and proposed.

- **Keywords:** Contaminants of emerging concern; Pharmaceutical compounds; Occurrence; Municipal wastewater treatment plant; Removal efficiency; Mass balance analysis; Environmental risk; Regulations

Wasim Iqbal, Yuk Ming Tang, Ka Yin Chau, Muhammad Irfan, Muhammad Mohsin. *Nexus between air pollution and NCOV-2019 in China: Application of negative binomial regression analysis*. Pages 557-565.

On a global scale, the epidemic of the novel coronavirus (NCOV-2019) has become a major issue that is seriously harming human health and impairing the environment's quality. The current study examines the association between air pollution and NCOV-2019 in China, where cases of NCOV-2019 are correlated with deaths in public databases with data on air pollution tracked at multiple locations in different provinces of China. A negative binomial regression (NBR) model was applied to examine the difference between the number of people infected with NCOV-2019 and the number of deaths in

China. The findings show that, after population density regulation, there is a positive connection between air pollutants concentration (particularly nitrogen dioxide) and the number of NCOV-2019 cases and deaths. Furthermore, PM2.5 is the key cause of NCOV-2019 cases and deaths in China. The results indicate that a 1% increase in the average of PM2.5 was correlated with an increase of 11.67 % in NCOV-2019 cases and a rise of 18 % in NCOV-2019 deaths. We concluded that a slight rise in air pollution has caused the number of NCOV-2019 cases and deaths to increase dramatically. This research provides a basis for future policies affected by this pandemic in terms of health and pollution.

- **Keywords:** COVID-19; Air pollution; PM2.5; SO2; PM10; NO2; O3; Negative binomial regression

Feiran Chen, Bin Chen, Zhengqiu Zhu, Yiduo Wang, Yong Zhao, Yatai Ji, Xiaogang Qiu, Quanjun Yin, Xiangjiang Xiao. *An extended area-partition-involved collaborative patrolling game in chemical clusters considering attackers' bounded rationality and parameter uncertainty*. Pages 567-577.

In our previous study—area-partition-involved collaborative patrolling (APCP) game, we proposed a cooperative patrolling game by utilizing multiple patrol vehicles to protect the chemical cluster. Except for fixed countermeasures like intrusion detection, the APCP game was proved to reduce the security risks of chemical clusters being attacked by terrorists effectively. However, some general assumptions (i.e., complete information game and perfect rational players) in the game model make it difficult to be applied in reality since the game model is not robust enough to deal with some common uncertainties on attackers. In this paper, we extend the APCP game model by considering the uncertainties of the game model from two aspects: (1) One is the bounded rationality of attackers. Attackers may adopt the ε-optimal response strategy without maximizing their payoffs strictly. In this circumstance, we propose the bounded rational APCP game solver. (2) The other is the uncertainties of the defender's estimation on the attacker's parameters. Some parameters regarding attackers are changed from exact values to distribution-free intervals. Correspondingly, we propose the interval APCP game solver. Through extensive simulations on a chemical cluster (i.e., the Antwerp Chemical Cluster), results of the case study indicate that when considering two types of uncertainties mentioned above, the defender's payoff will be slightly reduced, whereas the more robust patrolling routes are more easily convinced and adopted by the management department of chemical clusters and improve the process safety of chemical clusters.

- **Keywords:** Patrolling game; Chemical clusters; Bounded rationality; Parameter uncertainty; Game theory

Zhiyun Ji, Binbin Huang, Min Gan, Xiaohui Fan, Yifan Wang, Xuling Chen, Zengqing Sun, Xiaoxian Huang, Dan Zhang, Yong Fan. *Recent progress on the clean and sustainable technologies for removing mercury from typical industrial flue gases: A review*. Pages 578-593.

Mercury emitted from flue gas has been a typical kind of globally hazardous atmospheric pollutants. The efficient control is therefore significant for clean and sustainable industrial development. This paper focused on mercury emission behavior and the characteristics of typical industrial processes. Particularly, the work reviewed the control techniques and commented on the latest progress of harmless treatment techniques. It is found that non-ferrous metals smelting and coal combustion are the primary sources of atmospheric mercury, accounting for about 80 % of the total emissions. Compared with controlling mercury emission from the source and the process, the end-of-pipe treatment technologies were characterized by high efficiency, with removal rate of Hgp exceeding

90 %. During the flue gas purification process, mercury are merely separated, while the perniciousness is still existed. After heat treatment and plasma method, the mercury can be desorbed from the absorbents, through which the activity of adsorbents can be restored. Simultaneously, mercury can be purified into mercury by chelating agent, acid washing, and electrolysis, thereby realizing resource utilization. The paper also highlighted the advantages and constraints of emission control techniques, harmless and resourceful treatment. Moreover, some new ideas for the efficient disposal of mercury were provided.

- **Keywords:** Mercury; Industrial flue gas; Emission property; Controlling techniques; Resourceful treatment; Cleaner production