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Julio A. de Lira-Flores, Claudia Gutiérrez-Antonio, Richart Vázquez-Román. *A MILP approach for optimal storage vessels layout based on the quantitative risk analysis methodology*. Pages 1-13.

Abstract: The layout design for storage vessels is an important issue to keep safe process plants, since the accidents originated in storage areas are almost one-third of all reported accidents. In order to reduce fire and explosion damages different mathematical approaches have been proposed; however, most of them are not suitable for real storage facilities design. In this work, a MILP approach has been developed to find the optimal layout of storage vessels, seeking to minimize the cost associated with potential damage of fire and explosion. This approach allows allocation of suitable sites for storage vessels, reducing accidents propagation, and domino effect while keeping safety as much as possible the plant assets. In this way, the optimization approach provides substantial support for decision-makers during the design stage. The study case used to test the mathematical model considers 19 vessels, six buildings, five process facilities and 25 possible scenarios, which includes 16 fires and 9 explosions.

- **Keywords:** QRA; Storage facilities; Inherently safer design; Domino effect; MILP; Assignment problem

Bienvenu Mizero, Thresa Musongo, Eldon R. Rene, Ferdi Battes, Piet N.L. Lens. *Optimization of process parameters for the chemical leaching of base metals from telecom and desktop printed circuit boards*. Pages 14-23.

End-of-life electrical and electronic equipment are secondary sources of metals that can complement natural ores. Printed circuit boards (PCB) are an important resource from which base metals such as Cu, Ni, and Zn can be leached and recovered. Three types of PCB were studied: two boards from telecom equipment (T1 and T2) and one from a desktop with the aim to optimize the process parameter and determine the Cu, Ni and Zn content from T1, T2 and desktop PCB. Chemical leaching using sulphuric acid (H2SO4) and hydrogen peroxide (H2O2) was studied in batch reactors, upflow columns and stirred tank reactors (STR). The parameters optimized were pulp density (PD), H2SO4 and H2O2 concentration, stirring speed (RPM), and particle size for a contact time of 18 h. The optimum conditions for Cu, Ni and Zn leaching were: 4.3 M H2SO4, 4.8 M H2O2, 194 RPM, 0.1 (%, w/v) PD and 0.5 mm particle size. In batch conditions, a Cu leaching efficiency of 80% was achieved for PCB from T1, T2, and desktop. Furthermore, a maximum Cu recovery efficiency of 25.6 and 77.6% was obtained from T1 PCB in,

respectively, the upflow column and STR in 5 h for the particle size fraction 0.5–1.6 mm. T1 exhibited a higher metal content than T2 and desktop PCB. The smaller particle size, the high concentration of lixiviant and low PD increased the chemical leaching efficiency of Cu from PCB.

- **Keywords:** Chemical leaching; Telecom PCBs; Statistical optimization; Upflow column; Stirred tank reactor

Éva Farkas, Viktória Feigl, Katalin Gruiz, Emese Vaszita, Éva Ujaczki, Ildikó Fekete-Kertész, Mária Tolner, Csongor Márk Horváth, Zsófia Berkl, Nikolett Uzinger, Márk Rékási, Mónika Molnár. *Microcosm incubation study for monitoring the mid-term effects of different biochars on acidic sandy soil applying a multiparameter approach*. Pages 24-36.

Biochar is produced from organic materials by pyrolysis specifically for soil improvement. Interactions with beneficial outcomes between biochar and soil can arise within a short time but it is uncertain whether the effects are similar in all soil types and at different time-scale. The objective of this study was to evaluate the short-term and mid-term effects of biochars from different feedstocks (grain husks and paper fibre sludge, post-treated grain husks and paper fibre sludge, woodscreenings) on the soil physico-chemical, biological and ecotoxicological properties. As part of a complete scale-up technology, aiming improvement of an acidic sandy soil, a 12-month microcosm experiment was conducted with combined application of biochars, compost and fertilizer. The applied multiparameter approach made possible the selection of the most optimal treatment. All the three biochars had favourable influence on the soil, but the effects were different in terms of extent and time. Although the biochar from woodscreenings had not the most promising short-term effects, but combined with fertilizer at 0.5 w/w% biochar rate it was the most favourable treatment after 12 months. The grain husk and the paper fibre sludge biochar at 1 w/w% rate could also efficiently improve soil parameters and functions.

- **Keywords:** Acidic sandy soil; Biochar; Integrated monitoring; Mid-term assessment; Multiparameter approach; Soil improvement

Sophia Tsoumachidou, Apostolos Antoniadis, Ioannis Poulios. *Artificial and solar photocatalytic mineralization of psychoactive drugs-loaded urban wastewater: Inorganic ions and phytotoxicity assessment*. Pages 37-44.

The presence of psychoactive substances and/or their metabolites is confirmed, not only in urban wastewater, but also in aquatic plants and animal tissues, underlining the possible consequences for human health and ecosystems balance. As a alternative to conventional wastewater treatment methods, Advanced Oxidation Processes (AOPs) have received considerable attention for the treatment of water and wastewater contaminated with a wide variety of toxic pollutants. In this work, photocatalytic oxidation has been applied to simulated wastewater loaded with psychoactive drugs duloxetine and fluvoxamine under artificial and solar illumination, so that process effectiveness unto urban wastewater mineralization could be evaluated. The effects on the process' efficiency of TiO2 P25 catalyst's concentration, initial concentration of H2O2 and Fe3+, pH of the solution, as well as the type of radiation, were evaluated in a bench-scale Pyrex reactor and a scaled-up solar reactor. The treatment efficiency has been followed through the evolution of the organic matter content expresses as dissolved organic carbon (DOC). Moreover, the release of inorganic ions and the decrease in phytotoxicity of the simulated wastewater has been observed after solar-induced photocatalytic treatment.

- **Keywords:** Photocatalytic oxidation; Urban wastewater; Psychoactive drug; TiO2; Photo-Fenton; Solar

Kai Zheng, Minggao Yu, Ligang Zheng, Xiaoping Wen. *Comparative study of the propagation of methane/air and hydrogen/air flames in a duct using large eddy simulation*. Pages 45-56.

The propagation of methane/air and hydrogen/air explosion flames in four closed ducts with different aspect ratios was numerically investigated using large eddy simulation (LES). The numerical model was validated by comparing the numerical results with the experimental results, and reasonable agreement is observed between them. For methane/air, only the tulip shaped flame (concave flame front) can be observed after the flame inverts and no oscillation occurs. The tulip lips distortion occurs in the duct with aspect ratio (the ratio of length to width) of 7.5 in hydrogen/air, and the deformation becomes more distinguished as the aspect ratio increases. Consistent with the flame structure evolution, the flame speed and rate of pressure rise decrease after the flame touches the sidewalls in methane/air. For hydrogen/air, with the emergence of tulip lips distortion, an oscillation appears in the flame propagation speed and pressure curves when the aspect ratio is 7.5. Moreover, the oscillation becomes stronger as the aspect ratio increases. With this increase in the aspect ratio, the interaction between flame and pressure wave leads to the emergence of different flow patterns after the tulip shaped flame formation.

- **Keywords:** Methane/air; Hydrogen/air; Large eddy simulation; Flame propagation

Hamdi A. Al-Jamimi, Sadam Al-Azani, Tawfik A. Saleh. *Supervised machine learning techniques in the desulfurization of oil products for environmental protection: A review*. Pages 57-71.

Desulfurization, known as the removal of sulfur from oil, is extremely important in the petroleum processing industry and in the environmental protection. Several oil-upgrading processes such as desulfurization and catalysts such as alumina loaded with molybdenum have been proposed to deal with the problem of removing sulfur-containing compounds from light oil. Thus, several parameters are required to be experimentally optimized which demands a lot of work including reagents. Advanced mathematical tools can be used to optimize the desulfurization process and to study the related factors. The modeling and simulation of the desulfurization process have been proposed in several studies in order to facilitate a better understanding of the process operations. Machine Learning (ML) is regarded as a promising methodological area to perform such optimization and analysis. This review describes the relevant methods for dealing with the applications of ML for desulfurization in oil. Although a good number of research papers have appeared in recent years, the application of ML for desulfurization is still a promising area of research. The review presents an overview of the ML methods and their categories in desulfurization. It discusses and compares the methods that employ ML to optimize the desulfurization process. The review also highlights the findings and possible research directions.

- **Keywords:** Machine learning; Prediction model; Computational intelligence; Desulfurization; Sulfur contents

R. Felisberto, M.C. Santos, S. Arcaro, T.M. Basegio, C.P. Bergmann. *Assessment of environmental compatibility of glass–ceramic materials obtained from galvanic sludge and soda–lime glass residue*. Pages 72-78.

In this study, we evaluated the environmentalcompatibility of glass–ceramic materials produced from galvanic sludge and soda–lime glass to understand the occurring phenomena in the investigated ceramic system and to find an environmentally compatible way to recycle the materials. The formulated compositions were homogenised (with 1, 5, 10, and 20 wt% of galvanic sludge), compacted, and fired at various temperatures (750–1050 °C). The chemical composition, particle size, thermal behaviour, structure (via X-ray diffraction (XRD), and microstructure (via SEM) of the raw materials, samples, and obtained glass–ceramic materials were evaluated. The ceramic materials were submitted to leaching and solubilization assays. We successfully produced environmentally compatible ceramic bodies using the formulations with 1 and 5 wt% galvanic sludge. Harmful elements could be successfully immobilised. The findings are significant mainly when extended to the industrial scale where the strategic reuse of this waste type is a concern.

- **Keywords:** Galvanic sludge; Immobilization; Environmental compatibility

Muhammad A. Suleiman, Taoreed O. Owolabi, Hayatullahi Bolaji Adeyemo, Sunday O. Olatunji. *Modeling of autoignition temperature of organic energetic compounds using hybrid intelligent method*. Pages 79-86.

Autoignition temperature (AIT) plays a significant role while characterizing the potential hazard of energetic chemical compounds and occurrence of fire disasters can be easily managed and controlled through adequate knowledge of autoignition temperature of the compounds. However, the experimental determination of autoignition temperature is laborious and consumes appreciable time and resources. This present work addresses the challenges using hybrid support vector regression (SVR) and gravitational search algorithm (GSA) for precise modeling of autoignition temperature of organic energetic compounds using only molecular weight, as well as the number of hydrogen, oxygen and carbon atoms as descriptors. Apart from the superior performance of the proposed hybrid model (SVR-GSA) as compared with the existing models, the absence of specific functional groups of the energetic compound as descriptor further eases the applicability of the model. On the basis of mean absolute error between the estimated autoignition temperatures and the experimentally measured values, the proposed SVR-GSA model outperforms Mohammad et al and Chen et al model with performance improvement of 37.34% and 79.05%, respectively. Implementation of the proposed model would definitely ease autoignition temperature determination of energetic compounds and ultimately reduces the potential risk associated with these compounds while handling.

- **Keywords:** Autoignition temperature; Energetic compounds; Support vector regression and gravitational search algorithm

Juncheng Jiang, Hao Wu, Lei Ni, Mengya Zou. *CFD simulation to study batch reactor thermal runaway behavior based on esterification reaction*. Pages 87-96.

Thermal runaway is a hazardous problem frequently occurring in the chemical productions. An effective way to avoid accidents caused by thermal runaway is preliminary hazard analysis which can help determine the comparatively safe operating condition in the design phase. In this paper, a series of batch reactor thermal runaway scenarios based on esterification of isopropyl propionate has been studied and according to mixing law the optimal inhibitor injection location has been confirmed. The reactor model is established by computational fluid dynamics (CFD) technology and verified by RC1e test. The effect of cooling temperature, cooling velocity and stirring speed are investigated in detail. Based on the failure status analyses, the appropriate location of temperature probe was then determined by the divergence (DIV) criterion. Finally, the

inhibitory mixing performances were evaluated by a global mixing criterion. The results indicated the mixing time and inhibitory region were greatly influenced by the injection location.

- **Keywords:** Thermal runaway; Esterification reaction; Batch reactor; CFD

Shunyao Wang, Xu Peng, Sen Yang, Huabo Li, Jun Zhang, Liping Chen, Wanghua Chen. *Numerical and experimental studies on decomposition and vent of di-tertbutyl peroxide in pressure vessel*. Pages 97-106.

Study of thermal decomposition and vent of di-tertbutyl peroxide (DTBP) is beneficial for accidents prevention in chemical engineering. In order to deep understand the thermal decomposition and vent behaviors of DTBP in a pressure vessel, both computational fluid dynamics (CFD) simulation and pressure vessel tests (PVT) were carried out. Based on the DTBP decomposition kinetics evaluated from differential scanning calorimeter (DSC) experiments, CFD numerical simulation was performed to reveal the fluid dynamic behaviors, temperature profile and flow field during the thermal decomposition and vent processes. PVT experiments were conducted to validate the numerical model. The results showed that the simulated and experimental data were in good agreement, thereby proving the validity of the numerical model and the DTBP decomposition kinetic model.

- **Keywords:** Thermal; Decomposition; Vent process; Pressure vessel test; Computational; Fluid dynamics; Di-tertbutyl; Peroxide

R.A. Mesquita, R.A.F Silva, D. Majuste. *Chemical mapping and analysis of electronic components from waste PCB with focus on metal recovery*. Pages 107-117.

This paper describes a detailed chemical characterization of connector pins separated from diverse electronic components removed from waste printed circuit boards (WPCB) of computers. Chemical maps by SEM-EDS (Scanning Electron Microscopy - Energy Dispersive Spectroscopy) indicated that the substrates of all connector pins are made by Cu-Sn, Cu-Zn or Cu-Sn-Zn alloys, which are covered by thin Ni and Au layers. The ICP-OES (Inductively Coupled Plasma - Optical Emission Spectrometry) analysis of the different connector pins revealed that these materials are mostly constituted by Cu (62–88% w/w) and very attractive Au contents were found (up to 1273 g/t). For all pins, intermediate contents of Zn, low contents of Ni, Sn and Pb and very low contents of Pd and Fe were determined. A heterogeneous, 100% metallic sample was prepared by mixing all individual connector pins aiming at contribute to the development of feasible technologies for recovering valuable metals. The mixed sample contains about 73% w/w Cu and 168 g/t Au, which are higher than the contents reported in the literature for samples obtained after grinding assembled or disassembled WPCB. The leaching of the mixed sample without grinding and concentration steps will reduce operating costs and maximize metals recovery avoiding mass losses.

- **Keywords:** E-waste; Printed circuit boards; Electronic components; Characterization; Chemical mapping

Udayagee Kumarasinghe, Ken Kawamoto, T. Saito, Y. Sakamoto, M.I.M. Mowjood. *Evaluation of applicability of filling materials in permeable reactive barrier (PRB) system to remediate groundwater contaminated with Cd and Pb at open solid waste dump sites*. Pages 118-127.

This study aimed to identify appropriate filling materials for a permeable reactive barrier (PRB) system to treat groundwater contaminated with trace metals in the vicinity of solid waste landfills in Sri Lanka. Mixtures of alluvial loamy soil, coconut shell biochar, and

laterite clay brick in different proportions were tested as easily-available PRB adsorbents. A series of adsorption and desorption experiments were carried out to investigate the effects of initial concentration, pH, ionic strength, and multiple competitive trace elements on Cd and Pb adsorption onto the tested adsorbents. In addition, hydraulic conductivities (Ks) of the tested adsorbents under different compaction levels were measured to examine a suitable packing condition for the PRB system. Results showed that the Langmuir model performed well for fitting Cd and Pb adsorption isotherms and maximum adsorption capacities (Qm) for Pb (2.1–15.3 mg/g) became higher than those for Cd (0.8–6.8 mg/g). All tested adsorbents showed low leaching of adsorbed metals with high hysteresis indices in desorption studies. In the multiple trace element solution, the existence of other trace metals (Cu, Zn, Ni) had a significant effect on Cd adsorption but less on Pb adsorption. The three mixed adsorbents had no dependency on the initial pH and ionic strength of the solution, while the single material showed a low dependency in both Cd and Pb adsorption. The inclusion of brick was effective to improve the hydraulic property and measured Ks values for the 75% brick mixed materials resulted of >10−4 cm/s at high compaction levels (Dr = 90% and 100%). Three mixed materials can be strongly recommended as a PRB filling material to treat landfill leachate based on their reactivity and hydraulic properties.

- **Keywords:** Groundwater; Permeable reactive barrier (PRB); Adsorption; Desorption; Heavy metals; Hydraulic conductivity

A. Rahman Roshanida, Fakhru'l-Razi Ahmadun, Hind F.A. Barghash, Mimi Haryani Hassim. *Liquid state bioconversion continuous bioreactor of sewage sludge treatment: Determination and evaluation of mixed fungi growth kinetics*. Pages 128-135.

Liquid state bioconversion (LSB), a bioremediation and biodewatering process was applied for sewage sludge treatment in this study. The LSB process is a non-hazardous, safer and environmentally friendlier method for ultimate sludge management and disposal compared to the other available technologies. The system presented in this study was developed by using mixed fungi of Aspergillus niger and Penicillium corylophilum to treat sewage sludge in a LSB bioreactor. This research was conducted in order to study the LSB process on continuous system in terms of kinetic coefficients determination. For the continuous LSB process, a mathematical model was developed from the basic principles of material balance based on Monod equation. By investigating the kinetics of substrate utilisation and biomass growth, the kinetic coefficients of growth yield coefficient (Y), specific microorganism decay rate (Kd), half saturation constant (Ks) and maximum specific growth rate (μmax) were found to be 0.79 g VSS g COD−1, 0.012 day−1, 1.78 g COD L−1 and 0.357 day−1, respectively.

- **Keywords:** Sewage sludge; Kinetic coefficients; Continuous bioreactor; Aspergillus niger; Penicillium corylophilum; Bioremediation; Dewaterability

E.N. Dragoi, Zs. Kovács, T. Juzsakova, S. Curteanu, I. Cretescu. *Environmental assesment of surface waters based on monitoring data and neuro-evolutive modelling*. Pages 136-145.

The surface water quality highly depends on the natural conditions and on the industrial, agricultural and other anthropogenic activities in the river catchment areas. The quality of the surface water is the key factor in the water quality management. The monitoring of the water quality indicators is requested to follow up (in time and space) the changes in the water quality, providing healthy water for the people. The water quality indicators (physical-chemical specific parameters such as: pH, electrical conductivity, dissolved oxygen, turbidity etc.) provide information about the pollution degree of different waters (stemming from wastewater treatment plants, precipitation, sewer lines, tributaries,

etc.). The main aim of the research was to demonstrate the efficiency of artificial intelligence techniques for the water quality prediction. Consequently, the considered system was modelled using a neuro-evolutive technique, combining artificial neural networks (ANN) with differential evolution (DE) algorithm. The neural network acts as a system model, while the differential evolution algorithm is the optimizer with the function to determine the optimal parameters of the model. The simulation results pointed out that the approach is suitable to set up adequate models for the three parameters, pH, electrical conductivity, dissolved oxygen, respectively. For the fourth parameter (turbidity), an average absolute error of 30% was obtained, which indicates a more complex relation in rapport to the other parameters of the system. The DE-ANN approach can, thus, be further used in decision making solutions for water quality management.

- **Keywords:** Water framework directive; Surface water monitoring; Water quality assessment; Artificial neural networks; Differential evolution algorithm

Naushad Ahamad Ansari, Abhishek Sharma, Yashvir Singh. *Performance and emission analysis of a diesel engine implementing polanga biodiesel and optimization using Taguchi method*. Pages 146-154.

Diesel fuel emissions are the major source of air pollution and one of the main causes for the global warming worldwide. The present research is focused on the experimental study and input parameter analysis on polanga biodiesel blend, fuel injection timing, and fuel injection pressure on commonly used single cylinder 4-stroke direct injection diesel engine emissions (Unburnt Hydrocarbons-UHC, NOx, and smoke) and thermal efficiency at full load condition. In the study, the effect of polanga blends on fuel injection timing and fuel injection pressure is considered as input factors to examine engine output parameters and minimum exhaust emission is found with the blends of polanga biodiesel. As per the thermal performance evaluation, it is observed that the operating conditions of the engine with 30% polanga biodiesel blend at 220 bar injection pressure are similar to the operating conditions with diesel. Taguchi method has been adapted to obtain a rich design matrix for optimization of parameters. The engine's input parameters are optimized with multi-response characteristics of BTE, UHC, NOx and smoke. Multiple single-to-noise ratio (MSNR) is employed to analyze the performance characteristics from the actual value. In the study, the optimal values of BTE, UHC, NOx, and smoke emissions obtained are 32.59%, 20.3 ppm volume, 551 ppm volume, and 94.2% respectively at 30% polanga biodiesel blend with 15°bTDC fuel injection timing and 200 bar injection pressure.

- **Keywords:** Polanga biodiesel; Injection timing; Injection pressure; Taguchi method; Engine performance

Shuang Cai, Laibin Zhang, Jinqiu Hu. *Scale-reasoning based risk propagation analysis: An application to fluid catalytic cracking unit*. Pages 155-165.

When a disturbance occurs in a complex large-scale system, it may affect downstream equipment and several other process variables to evolve into a larger risk. The connectivity of process equipment may make it difficult to identify the propagation path of the disturbance. Understandably, the root cause identification of widespread disturbances gets its share of attention from researchers for remedial action but the prediction of the propagation path to prevent widespread disturbance is often overlooked. The scale-reasoning based risk propagation analysis method is proposed in this paper to predict the probable propagation path so that corrective actions can be taken in time to avoid further loss. By dividing the spatial scale of a complex production system, the approach uses transfer entropy to find the causal relationship between process variables and establish the risk propagation scale-reasoning model in the form of a causal map; then the risk propagation searching method, based on kernel extreme learning machine,

is used to forecast the risk propagation path. An actual industrial case is analyzed to illustrate the effectiveness of the proposed method.

- **Keywords:** Multi-scale; Scale-reasoning; Transfer entropy; Propagation path

Elham Mir, Hamed Rashidi, Peyvand Valeh-e-Sheyda. *Towards a CFD-based analysis of a full-scale sludge tank to enhance dewatering capacity of the downstream filter press*. Pages 166-177.

A computational fluid dynamics (CFD) model was developed for sludge mixing-settling in a laboratory scale sludge tank based on the Takács exponential function. A dynamic experimental program was also undertaken at different rotational speeds of mixers and the concentration of sludge to validate the sludge sump model. The deviation between the simulated interface height and the experimental data was 2%. The validated CFD model was then employed to develop a novel operating methodology for operation of a full-scale sludge tank. The proposed model includes two consecutive periods of sludge mixing and settling, resulting in reducing the mixers' working time. In the current operating mode, the energy consumption of mixers has been reduced by 91.67%. Based on the two-phase, 3-D modeling results of the sludge tank, the post-construction sludge tank is simultaneously able to act as a secondary clarifier, as well as a storage tank. As a key finding of the study, the treatment capacity of the filter press in downstream has accelerated, so that the working hours and energy consumption of the filter press has been improved by 55%.

- **Keywords:** Computational fluid dynamics; Settling velocity; Mixer; Sludge tank; Energy consumption

Muhammad Athar, Azmi Mohd Shariff, Azizul Buang, Heri Hermansyah. *Inherently safer mechanical material selection for process equipment*. Pages 178-186.

Hazards associated with chemical processes can lead to accidents, which can be managed through process safety strategies. Inherent safety is a proactive tactic, capable of both identifying and minimizing the hazard. Available inherent safety assessment (ISA) methods focus on route selection only. Individual process equipment characteristics, especially the mechanical aspects are not reported for ISA. Subsequently, this paper presents a new technique for suitable material selection of process equipment at initial design stages. In inherently safer mechanical material (ISMM), process characteristics are coupled with the mechanical attributes for mechanical material selection of process equipment. The relative ranking of process equipment is used to highlight the critical process equipment that is more prone to leak. This risky process unit is further studied to select the suitable mechanical material. Two-fold mechanical compatibility criteria are established, which needs to be satisfied for material selection. If the proposed material is found unsuitable, inherent safety theme is used to propose the suitable material. The ISMM technique is verified by a case study of MMA-TBA process plant Hysys simulation. The technique is simple and identifies the crucial equipment in early design stages, which can help the design engineers to implement inherent safety at the basic design stage.

- **Keywords:** Basic design engineering; Indexing; Inherent safety; Mechanical material; Process simulation

Tianlong Zheng, Peng Li, Xiaoyu Ma, Xiaohong Sun, Chuanfu Wu, Qunhui Wang, Ming Gao. *Pilot-scale multi-level biological contact oxidation system on the treatment of high concentration poultry manure wastewater*. Pages 187-194.

A pilot-scale (5 m3/d) study was applied for the treatment of a high-strength poultry manure wastewater by using a multi-level biological contact oxidation tanks system with novel carriers. Firstly, four kinds of carriers including porous block carriers, sponge globoid carriers, fiber ball carriers, and suspend plastic carriers were compared at lab-scale experiment to choose the best performed carriers for the further application in pilot scale experiment. Then, the performance of the pollutants elimination during the whole pilot-scale reactor as well as the contribution efficiency of each tank under different influent pollutants loads were investigated. Finally, the biomass evaluation on the carriers and the mechanism of nitrogen removal were also explored. The conclusion showed that the effluent quality could satisfy the discharge standard of pollutants for livestock and poultry breeding industry (GB 18596-2001) when the influent organic load was less than 3.64 kg CODcr/(m3 d) during the pilot-scale system placed with the porous block carriers. The contact oxidation tank I dominated the average contribution efficiency of CODcr (89.2%), ammonia (69.6%), and the total nitrogen (57.3%) during the three-level biological contact oxidation tanks. The step-feed operational model was suggested to further increase the pollutants removal capacity of the following Tank II and Tank III. The oxygen-deficient environment of the biofilm and the proper three-dimensional spiral structure of the carriers were suitable for the happening of the simultaneous nitrification and denitrification occurred in the pilot-scale aerobic reactor.

- **Keywords:** Multi-level biological contact oxidation tanks; Porous block carriers; Poultry manure wastewater; Simultaneous nitrification and denitrification (SND)

Martín M. Dávila-Jiménez, María P. Elizalde-González, Mario A. Guerrero-Morales, Jürgen Mattusch. *Preparation, characterization, and application of TiO2/Carbon composite: Adsorption, desorption and photocatalysis of Gd-DOTA*. Pages 195-205.

The preparation methodology of a photocatalytic acting composite consisting of TiO2/Carbon carrying 24.5% of TiO2 is described. The environmental friendly TiO2/Carbon bifunctional material combining immobilized photocatalytic properties with a macroparticular carbonaceous ad-/desorbent was prepared in one-step procedure at low temperature from guava seeds and Ti(IV) oxysulfate as carbon and photocatalyst precursors, respectively. With artificial solar radiation, the composite can act as a photocatalyst for the degradation of the emerging pollutant, gadolinium-based contrast agent Gd-DOTA in aqueous solution with a degradation yield of 95%. For its reuse, the composite can be separated from the solution without centrifugation. The TiO2/Carbon composite is also able to adsorb and desorb the non-complexed gadolinium (Gd3+) ion once the cyclic Gd-DOTA is destroyed. The resulting photodegradation /-transformation as well adsorption and desorption phenomena were studied by analyzing the occurring Gd-species using ion exchange chromatography coupled to element and molecule selective mass spectrometers on-line (IEC-ICP-MS/ESI-QToF-MS).

- **Keywords:** Photocatalyst; TiO2; Adsorbent; Carbon; Gadolinium complex; Photoproducts of DOTAREM; IC-ICP-MS/ESI-QToF-MS

Qianlin Wang, Laibin Zhang, Jinqiu Hu. *Real-time risk assessment of casing-failure incidents in a whole fracturing process*. Pages 206-214.

With the increasing development of hydraulic fracturing technologies, shale gas exploitation is becoming a highly industrial process. Casing-failure incidents which could cause serious leakage of the high-pressure and hazardous chemicals have triggered an intense public discussion in the fracturing industry. Quantitative risk analysis (QRA) is a common technique used to study the carrying capacity of a casing. However, this technique tends to only show static risk state after the casing has been run down to the formation, but is not sufficient to monitor its real-time failure risk during the whole fracturing process. Therefore, a matrix-based risk assessment method is proposed to

improve the conventional QRA by using stress-strength interference theory and value function modelling to calculate the static and dynamic failure probabilities of casings, respectively, over a period of multi-stage sand fracturing. Further studies are developed to integrate these two probabilities with the application of a design matrix, particularly for the quantitative analysis and assessment of casing failures. The visual risk graphs are also provided to show the failure risk states and levels for the casings in real time. The assessment procedures can clearly delineate the operation characteristics of shale gas fracturing – high pressure, large displacement, and sand erosion. To illustrate the validity of the methodology, a production casing of a gas well at one fracturing stage is chosen as a test case. Results show that the real-time risk is more accurate and practical, as well as improving the assessment effectiveness of casing-failure incidents during a whole fracturing period.

- **Keywords:** Casing failure; Real-time risk assessment; Shale gas fracturing; Risk matrix; Design matrix

Chris T. Cloney, Robert C. Ripley, Michael J. Pegg, Faisal Khan, Paul R. Amyotte. *Lower flammability limits of hybrid mixtures containing 10 micron coal dust particles and methane gas*. Pages 215-226.

Mixtures of combustible dust and flammable gas pose an increased explosion risk in processing equipment due to reduced flammability limits over the dust and gas alone. Although correlations have been proposed based on experimental testing for predicting the flammability limits of hybrid mixtures from those of the dust and gas, none appear to be applicable across a range of fuel mixtures. The objective of this work is to use computational fluid dynamics to explore the lower flammability limits of 10μm coal dust particles and methane gas under laminar, free-flame conditions, and to compare the limits to the experimentally determined mixing rules. This comparison gives an understanding of the baseline behaviour upon which different fuel mixtures, equipment geometry, and various operational conditions can be added in the future. The results from the computational model suggest that Le Chatelier's Law, which proposes linear mixing between the dust and gas limits, is applicable for the small particles studied. Bartknecht's curve, which proposes wider flammability limits than linear, appeared to be overly conservative, while new relations that predict narrowing of the limits did not appear to delineate flammable mixtures under the conditions investigated.

- **Keywords:** Lower flammability limit; Coal dust; Methane gas; Hybrid mixtures; Laminar flame propagation

Omar S. Baghabra Al-Amoudi, Ammar M. Alshammari, Saad A. Aiban, Tawfik A. Saleh. *Volume change and microstructure of calcareous soils contaminated with sulfuric acid*. Pages 227-236.

Acid contamination of soils is a common problem within fertilizer and petrochemical industries. Soil properties could be altered due to acid contamination, especially the volume change within the vicinity of the contaminated soils. There are huge petrochemical and fertilizer industries in the industrial areas that produce or utilize different acids. Further, most of the soils used for road bases and under pavement and walkways are calcareous in nature. These carbonate soils are susceptible to large volume change when attacked by acids. This research aims to study the volume and microstructural changes using two calcareous soils, i.e. non-plastic and plastic marls, due to interaction with sulfuric acid at three different concentrations. The soil samples were prepared in high-density polyethylene (HDPE) molds that were placed in large containers and instrumented with linear variable differential transformer (LVDT) to measure the volume change. The morphology and composition analyses were studied utilizing scanning electron microscopy and X-ray diffraction. Results of this investigation indicate that the volume change and acid concentration were proportional except in the case with

the non-plastic marl at high acid concentration. This was ascribed to the severe reaction of sulfuric acid with the carbonate minerals resulting in blocking the paths for further infiltration of the acid into the whole soil.

- **Keywords:** Soil pollution; Sulfuric acid; Volume change; Contamination; Calcareous soils; Mechanism

Shuaiwei Gu, Yuxing Li, Lin Teng, Qihui Hu, Datong Zhang, Xiao Ye, Cailin Wang, Jinghan Wang, Stefan Iglauer. *A new model for predicting the decompression behavior of CO2 mixtures in various phases*. Pages 237-247.

The pipeline transportation has been considered as the best way to transport pressurized CO2 and plays an important role in Carbon Capture and Storage (CCS) technology. The risk of ductile fracture propagation increases when a CO2 pipeline is ruptured or punctured, and CO2 decompression behavior must be determined accurately in order to avoid the catastrophic failure of the pipeline and to estimate the proper pipe toughness. Thus in this work, a new decompression model based on GERG-2008 equation of state was developed for modeling the CO2 decompression behavior. And for the first time, a relaxation model was implemented to calculate the sound speed in two-phase region. The model predictions were in excellent agreement with experimental 'shock tube' test data in the literature. Furthermore, via modeling, it has been demonstrated how impurities in the CO2 and initial temperatures would affect the CO2 decompression wave speed in various phases. The results obtained show that the effects of these factors on supercritical and gaseous CO2 mixtures are absolutely different while liquid CO2 mixtures behave very similarly when compared to supercritical CO2 mixtures, which indicate that the toughness required to arrest fracture propagation is highly based on the initial phase states of CO2 fluid.

- **Keywords:** CO2 pipelines; Decompression wave speed; CO2 mixtures; Fracture propagation control; Equation of state

Reza Parand, Dominic C.Y. Foo, Raymond E.H. Ooi, Raymond R. Tan, Jui-Yuan Lee. *An algebraic targeting approach for optimal planning of gas sweetening problem in non-conventional gas field development*. Pages 248-255.

An algebraic technique based on pinch analysis has been developed for the planning of non-conventional natural gas (NG) field development projects. The development of NG fields with high carbon dioxide (CO2) content has become increasingly common in the oil and gas industry. In such cases, the raw NG needs to be treated in situ for CO2 removal to meet the sales gas specifications before being sent to the onshore gas processing plants (GPPs). The captured CO2 can either be reinjected into the reservoir for permanent storage, or utilised for enhanced oil recovery (EOR), for which partial sequestration may also be achieved. These options create the need to develop systematic techniques to provide high-level decision support for field development planning. The algebraic technique developed in this work overcomes the limitations of a recently developed graphical technique (Foo et al., 2016), as it relaxes the previous simplistic assumptions on stream purity requirements. Two case studies are used to illustrate the methodology.

- **Keywords:** Process integration; Pinch analysis; Composite table algorithm (CTA); CO2 capture

Khairulnadzmi Jamaluddin, Sharifah Rafidah Wan Alwi, Zainuddin Abdul Manan, Khaidzir Hamzah, Jiří Jaromír Klemeš. *Hybrid power systems design considering safety and resilience*. Pages 256-267.

Hybrid power systems are becoming more popular nowadays as they provide a good transition towards renewable energy systems integration while still maintaining power sources from fossil fuels. Uncertainties based on seasonal changes, weather patterns and demand fluctuations have been considered. Disasters such as earthquake, tornado and hurricane are becoming more frequent and unpredictable as climate change is affecting major parts of the world. Safety and resilience are two important aspects that need to be taken into consideration in designing power systems due to the increase in extreme weather and natural disasters. Safety precautions are taken into consideration to withstand major damage and ensure the power system can continue to run smoothly with no or little interruption to the power supply. Previous studies focused on optimizing the cost and efficiency of the system based on season change, weather and demand fluctuations. The purpose of this research is to develop a novel methodology to design a hybrid power system considering resilience and safety aspects. This research primarily focuses on the use of Decision Matrix Risk Assessment Technique (DMRA) and Power Cascade Table (PCT) to evaluate the impact of disasters towards the power systems with and without safety consideration. The results of the case study have shown that the implementation of safety can reduce the total cost by up to USD209.3 M when catastrophic events occur.

- **Keywords:** Power Pinch Analysis; Hybrid power system; Safety; Resilience; Catastrophic events

Urszula Kotowska, Joanna Karpinska, Justyna Kapelewska, Ewa M. Kowejsza, Alicja Piotrowska-Niczyporuk, Janina Piekutin, Adam Kotowski. *Removal of phthalates and other contaminants from municipal wastewater during cultivation of Wolffia arrhiza*. Pages 268-277.

The usefulness of Wolffia arrhiza for decontamination of waters from phthalates and other organic compounds was studied using artificial growing medium and real municipal wastewater samples. The eight most frequently detected phthalates were considered: dimethyl (DMP), diethyl (DEP), dipropyl (DnPP), dibutyl (DnBP), diisobutyl (DIBP), bis(2-ethylhexyl) (DEHP), diizoheptyl (DIHP) and diizononyl (DINP). The reduction of phthalates concentration observed during seven days of W. arrhiza cultivation on artificial growing medium was between 78.9 and 99.7%. Kinetics of phthalates degradation by W. arrhiza in real effluent wastewater was similar to those with laboratory-made solutions. The significant removal of nutrients (75–78%) and reduction of oxygen demand (93–97%) was achieved during cultivation of W. arrhiza. Purification efficiency of non-treated municipal wastewater with W. arrhiza was better than obtained with the use of Lemna minor, which is wide used in constructed wetlands, and not much worse than those obtained in conventional Wastewater Treatment Plant (WWTP). Analysis of biochemical components, stress markers and antioxidant activity in W. arrhiza shows its good acclimation to high pollution of aquatic environment.

- **Keywords:** Wolffia arrhiza; Lemna minor; Phytoremediation; Phthalates; Municipal wastewater

Q. Xu, G. Siracusa, S. Di Gregorio, Q. Yuan. *COD removal from biologically stabilized landfill leachate using Advanced Oxidation Processes (AOPs)*. Pages 278-285.

The removal of soluble organic matter from mature landfill leachate by means of biological, chemical, and combined biological-chemical methods was investigated in this

study. Aerobic sequencing batch reactor (SBR) with activated sludge was used as the biological treatment to remove ammonium. The chemical treatments included ozone (O3), ozone + hydrogen peroxide (O3 + H2O2), Fenton's reagents (H2O2 + Fe2+), and ozone + Fenton's reagents (O3 + H2O2 + Fe2+). Results indicated that the SBR achieved approximately 25% Chemical Oxygen Demand (COD) removal with an initial COD of 1276 mg/L. Ozonation of raw leachate achieved 16% COD removal after 240 min of treatment while O3 + H2O2 achieved 33% COD removal of raw leachate with 900 mg/L H2O2 in 120 min. Moreover, Fenton's process also achieved 33% COD removal from raw leachate. Results suggest that the biological treatment followed by chemical treatments had the most efficient COD removal. After biological stabilization, ozonation removed 52% of the COD within 240 min. The Fenton's process achieved 67% COD removal using equal doses of H2O2 and Fe2+. However, Fenton's reagents in conjunction with O3 removed 69% and 72% COD in 120 min and 240 min, respectively. The dosage test also revealed that the 2:1 ratio of H2O2 and Fe2+ had the best COD removal. Therefore, these results indicate that the combination of biological and post-chemical treatment methods effectively remove organic pollutants from mature landfill leachate.

- **Keywords:** Landfill leachate treatment; COD removal; Advanced Oxidation Processes; Aerobic SBR; Ozonation; Fenton's reagents

Bing Wang, Feng Qian. *Three dimensional gas dispersion modeling using cellular automata and artificial neural network in urban environment*. Pages 286-301.

The gas dispersion simulation in complex urban environment posts challenges on consequence analysis. Though computational fluid dynamics (CFD) are general approaches to provide building-resolving estimates, the time consuming calculation and complex process of modeling limit their application for emergency response. In this paper, a cellular automata dispersion model is prompted to simulate continuous point release of propane in 3-D domain with ground obstructions. An artificial neural network is employed to calculate the temporal state transition of cellular automata. To provide data for the neural network to train, fire dynamic simulator (FDS) code is adopted to simulate 100 scenarios of propane release from a fixed position in pre-specific domain with different combinations of meteorological conditions and source parameters. A proportion of the simulation results is selected to train the artificial neural network with different transition rules derived from the advection-diffusion equation. The dispersion processes are eventually replicated with the proposed approach on the remaining scenarios that the artificial neural network has never encountered. Provided with detailed meteorological field data, the cellular automata model could calculate the gas dispersion process about 1.5 times faster than FDS. As to the model performance, in the long term evolution, decreases in model accuracy are observed due to the nature of cellular automata in explicit evolution and the unavailability of error compensation methods. The transition rule that takes source terms into consideration outperforms in estimating the concentration distributions.

- **Keywords:** Cellular automata; Artificial neural network; Consequence modeling; Fire dynamic simulators

Huaizhan Li, Guangli Guo, Nanshan Zheng. *Influence of coal types on overlying strata movement and deformation in underground coal gasification without shaft and prediction method of surface subsidence*. Pages 302-312.

Under the action of high temperature, the mechanical properties of coal will change significantly. After gasification, different types of coal will form different surrounding rock mechanical characteristics, which may have different impacts on the movement

characteristic of combustion space areas overlying strata and surface. Without considering the influence of coal types or degree of coalification, the actual underground coal gasification (UCG) projects may have issues, such as instability of surrounding rocks in the combustion space zones, damage to surface buildings and structures. At present, the surface subsidence prediction method for UCG and underground gasifier design haven't considered the effects of different coal types. Therefore, this paper studies the influence of coal types on the movement characteristics of the combustion space area overlying strata and surface through field measurement, theoretical analysis and numerical simulation. The research results are as follows: 1) The principle of the mechanical property change of different types of coal is different after UCG; 2) Different types of coal have an effect on the surrounding rock movement and deformation around combustion space area, the vertical stress distribution of coal pillar and the surface subsidence. The strong-caking coal underground gasification is more useful for controlling overlying strata movement in the combustion space area and reducing the surface subsidence; 3) The prediction method of surface subsidence for UCG without shaft is proposed and the method is applied to the Ulanqab UCG industrial experiment field; 4) Suggestions for the design of gasifiers and isolated coal pillars considering the impacts of different coal types are proposed. The research results have important guiding significance and practical value for underground gasifier and isolated coal pillar design, surface subsidence prediction and UCG industrialization development.

- **Keywords:** UCG without shaft; Overlying strata structures around combustion space areas; Different coal types; Subsidence prediction; Gasifier and isolated coal pillar design

Luca Fortunato, Nirenkumar Pathak, Zahid Ur Rehman, Hokyong Shon, TorOve Leiknes. *Real-time monitoring of membrane fouling development during early stages of activated sludge membrane bioreactor operation*. Pages 313-320.

Non-invasive analysis and a final destructive analysis were employed to study the fouling formation during the initial days of AS-MBR operation. The fouling layer development was quantified in-situ non-invasively with Optical Coherence Tomography (OCT). The increase in biomass thickness was related to the transmembrane pressure (TMP) and to the increase in concentration of soluble microbial products (SMP) in the reactor The OCT non-destructive analysis allowed normalizing the final autopsy values for the amount of biomass deposited on the membrane. After 8 days of operation, the cake layer presented a biomass activity of 400 pg/mm3 of intra-ATP and EPS concentration of 9.8 mg/ mm3. The microbial community analysis of sludge and biofouling on the membrane surface revealed the abundance of Proteobacteria.

- **Keywords:** Cake layer; Membrane fouling; Optical coherence tomography (OCT); Membrane autopsy; Microbial community

Seyyed Abbas Mirzaee, Neamat Jaafarzadeh, Sahand Jorfi, Helder T. Gomes, Mehdi Ahmadi. *Enhanced degradation of Bisphenol A from high saline polycarbonate plant wastewater using wet air oxidation*. Pages 321-330.

In the present study, wet air oxidation (WAO) was investigated for the decomposition of bisphenol A (BPA) in high saline polycarbonate plant wastewater (PCW). The main operating conditions of the WAO process that affects the degradation efficiency, including temperature, total air pressure and reaction time were studied. The results indicate that complete BPA degradation is achieved in pH 8.5, temperature = 150 °C, total air pressure of 3 MPa and 120 min. In addition, by prolonging the reaction time to 24 h, removals of 62% and 37%, were obtained regarding chemical oxygen demand (COD) and total

oxygen carbon (TOC), respectively. The intermediates of BPA degradation generated in aqueous solution by the WAO process were identified and the proposed plausible mechanism was reported. Under optimum experimental conditions, the biodegradability of treated PCW after WAO process was shown to significantly improve, by analysis of biodegradability index, including BOD5/COD ratio, values of average oxidation state (AOS) and carbon oxidation state (COS). The WAO process was found to be an effective method to degrade highly toxic organic matter in high saline industrial wastewater such as PCW. The results indicate that WAO, as a pretreatment technology, is an economic and eco-friendly method for the treatment of PCW.

- **Keywords:** Polycarbonate plant; Bisphenol A; Wet air oxidation; Biodegradability; High saline wastewater; Petrochemical wastewater

S.M. Tauseef, Tasneem Abbasi, V. Pompapathi, S.A. Abbasi. *Case studies of 28 major accidents of fires/explosions in storage tank farms in the backdrop of available codes/standards/models for safely configuring such tank farms*. Pages 331-338.

Twentyeight accidents involving major fires and/or explosions, which have occurred across the world in tank farms storing flammable liquids, have been studied. The focus has been on determining, a) what were the distances between the tank which failed and the tank(s) which were damaged or could have been damaged due to fire/explosion in the former; b) what were the distances prescribed as safe by prevailing codes/standards/models between the concerned tanks, and c) whether the tanks were relocated in a safer way by the concerned industry after the accident. The study also identifies some of the codes, standards, and models which appear to provide more realistic safe distances for the given tank types/sizes.

- **Keywords:** Flammable substances; Storage tanks; Fire; Explosions; Chemical process industry; Safe distances

R. Saravanan, Devaraj Manoj, Jiaqian Qin, Mu. Naushad, F. Gracia, Adam F. Lee, Mohammad Mansoob Khan, M.A. Gracia-Pinilla. *Mechanothermal synthesis of Ag/TiO2 for photocatalytic methyl orange degradation and hydrogen production*. Pages 339-347.

Photocatalysis offers a promising route to address the challenges of future energy production and anthropogenic environmental pollution. Here we demonstrated the synthesis of a high activity Ag/TiO2 photocatalyst through a two-step, sol-gel and mechanothermal decomposition method employing a silver acetate precursor. Bulk and surface characterization revealed the formation of dispersed metallic silver nanoparticles (~9 nm diameter) decorating anatase crystallites (~14 nm) which stabilized a significant concentration of Ti3+ surface species. Synergy between silver and titania enhanced the photophysical properties, narrowing the band gap and suppressing charge-carrier recombination. Ag/TiO2 exhibited good visible light activity and excellent stability over 3 cycles for the aqueous phase photocatalytic degradation of methyl orange dye (38 μmol/h/gcat), and excellent hydrogen production from water splitting (910 μmol/h/gcat).

- **Keywords:** TiO2; Silver; Photocatalysis; Hydrogen; Methyl orange

Soheil Sobhanardakani, Azadeh Jafari, Raziyeh Zandipak, Alireza Meidanchi. *Removal of heavy metal (Hg(II) and Cr(VI)) ions from aqueous solutions using Fe2O3@SiO2 thin films as a novel adsorbent*. Pages 348-357.

In this work, plasma-enhanced chemical vapor deposition method was used for synthesizing Fe2O3@SiO2 thin films as a novel adsorbent for removal of heavy metal mercury(II) and hexavalent chromium ions from water samples. To that end, crystalline structure, chemical state, morphology, optical and magnetic property of deposited film were characterized using X-ray diffractometry (XRD), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), UV–vis spectrophotometer (UV–vis), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and vibrating sample magnetometer (VSM) system respectively. Then, the effects of some parameters such as the initial pH, the initial content of metal, the synthesized adsorbent dose, the contact time, the temperature and the ionic strength were analyzed for a batch adsorption system. The adsorption data was modeled by different models using the origin nonlinear software version 6.1. The results indicated that, the adsorption kinetics was well fitted by the pseudo second-order model, while the adsorption isotherm was well fitted by the Brouers–Sotolongo model. Moreover, it was found that the maximum adsorption process capacities of metal ions on adsorbent were 335.5 8 mg g−1 for Hg(II) and 152.8 mg g−1 for Cr(VI). It was also noted that, the mechanism of adsorption was complex where several types of interaction between ions and the surface of the prepared adsorbent were involved. Also, based on the results of the desorption studies it was speculated that adsorbent could be easily regenerated using eluents.

- **Keywords:** Adsorption; Chromium; Fe2O3@SiO2 thin films; Mercury; Removal efficiency

Andrei Horvat. *CFD methodology for simulation of LNG spills and rapid phase transition (RPT)*. Pages 358-369.

Hazards related to transportation and storage of Liquefied Natural Gas (LNG) are widely studied due to an increasing importance of LNG in the overall energy supply. Large scale LNG spills on water are of particular interest as much of LNG transport is conducted by sea. The present work focuses on modelling approaches and their capabilities to predict different phenomena related to LNG spills. It describes in detail a developed CFD based methodology that is able to simulate the behaviour of LNG spills from their initial release, spreading on the water surface, Rapid Phase Transition (RPT) to subsequent dispersion. The methodology is based on a homogeneous multiphase formulation of the liquid layer and therefore suitable for implementation in most of commercial CFD packages. An LNG release from a process train on a FLNG vessel was used to demonstrate capabilities of the developed approach. A CFD simulation was conducted to calculate the volume and distribution of the flammable cloud, and the overpressure generated by an RPT event.

- **Keywords:** Computational fluid dynamics; Liquefied natural gas; Rapid phase transition; Boiling regime; Flammability limit; Cloud formation; Pressure load; Hazard study; Numerical simulation

Laibin Zhang, Xin Zhang, Jinqiu Hu, Huizhou Liu. *A comprehensive method for safety management of a complex pump injection system used for shale-gas well fracturing*. Pages 370-387.

A pump injection system used in the shale-gas well fracturing process is subjected to various adverse factors during its service, such as high pressures of up to 105 MPa and a large displacement, leading to a high failure rate and a rapid degradation in system performance. To ensure the safety and reliability of such a system, a comprehensive safety management method based on a dynamic object-oriented Bayesian network (DOOBN) is proposed in this article. The approach provides a framework that integrates a system function model, causal model, system behaviour model, and online fault diagnosis model with a remaining life prediction model, to characterise the behaviours in a complex system, such as fault propagation and system degradation. This method could achieve fault diagnosis and also predict the degradation trend of critical components and system

performance in the long term, starting from the current system state. The application of the integrated safety management approach to the specific example of the pump injection system demonstrates how each phase of the presented method contributes to the achievement of fault diagnosis and residual life prediction in a systematic and holistic way. It is shown that the proposed model is a reasonable starting point for forecasting the remaining life of pump injection systems. This approach could be integrated into a real-time safety warning device for field application.

- **Keywords:** Shale gas; Pump injection system; Dynamic object-oriented Bayesian network; Fault diagnosis; Remaining life prediction