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Gui Fu, Xuecai Xie, Qingsong Jia, Wenqing Tong, Ying Ge. *Accidents analysis and prevention of coal and gas outburst: Understanding human errors in accidents*. Pages 1-23.

Coal is an important energy resource internationally. However, accidents have severely restricted the clean and safe production of coal resources. Among such accidents, coal and gas outburst accidents are a kind of coalmine disaster with high destructive power. Previous research on coal and gas outburst accidents mainly focused on gas factors but ignored the role of human factors. This paper analyses the coal and gas outburst accidents in China from 2008 to 2018 and studies its macroscopic laws. To better understand the causes of coal and gas outbursts, this paper uses the 24modelel to analyse coal and gas accidents and suggest measures for accident prevention from the two aspects 'gas' (risk control) and 'humans' (behavioural safety). Macroscopic law research found the following: (1) March, May, July, and August are the predominant months for accidents. (2) The second to fourth hours of the working hours and the first hour before the end of work are the peak periods for accidents. (3) Guizhou, Hunan, Henan, Sichuan, Yunnan, and Chongqing are the provinces with the most coal and gas outburst accidents. (4) An overall 75.82 % of accidents occurred in the driving face, and 81.08 % of accidents occurred in coal and gas outburst mines. (5) Blasting, drilling, driving, and coal falling are the main inducing factors. Case analysis of accidents found the following: (1) Human error is the leading cause of accidents. Among the errors, the lack of strict enforcement of outburst prevention measures, illegal command, and the illegal operation of miners are the main unsafe acts. (2) Safety knowledge and awareness of miners is not generally high, and serious habitual violations and unsafe psychologies exist. (3) The gas comprehensive prevention system and supervision system in the coal mine safety management system (SMS) can be easily operated improperly, and the safety training system and emergency management system can be absent. (4) Coalmine enterprises seriously lack safety culture.

- **Keywords:** Coal and gas outburst; Accidents analysis and prevention; 24modelel; Human errors; SMS; Safety culture

Ayush Singh, Munish K. Chandel. *Effect of ageing on waste characteristics excavated from an Indian dumpsite and its potential valorisation*. Pages 24-35.

This paper assesses the effect of ageing on physicochemical characteristics of excavated municipal solid waste from Mulund dumpsite in Mumbai, India. Based on disposal year,

waste was excavated from different zones in the dumpsite. The excavated waste was screened into five different size categories and further sorted into different streams. Physicochemical characteristics, i.e., pH, bulk density, ultimate and proximate analysis, calorific value and heavy metal concentration of excavated waste were also determined. The results indicate a change in the characteristics and composition of waste with age. The particle size distribution of waste revealed that waste above 80mm was mostly plastic and textile, whereas <4mm (fine fraction) composed of soil-like material. Above 80mm fraction shows a decreasing trend with age and depth, suggesting particle size reduction with time. Parameters like volatile matter, total and organic carbon and calorific value of excavated waste also reduced with the age. A significant portion of waste was fine fraction (~45%) emphasising on its valorisation for success of landfill mining. Furthermore, metal content in the dumpsite was <1%. The findings from this study can be used to reclaim dumpsites and suggest possible valorisation routes for excavated waste in developing countries like India.

- **Keywords:** Physicochemical characteristics; Legacy waste; Remediation; Landfill mining; Municipal solid waste; Indian dumpsite

Yuntao Li, Doudou Xu, Jian Shuai. *Real-time risk analysis of road tanker containing flammable liquid based on fuzzy Bayesian network*. Pages 36-46.

The risk of road transportation of flammable liquid is of great uncertainty due to the time-varying conditions of the passing locations and the environment, which leads to challenging risk analysis. In this work, a real-time risk analysis method for road tanker transportation based on the fuzzy Bayesian network (FBN) is proposed. The bow-tie model is first employed to identify hazards in flammable liquid road transportation systems and shows risk evolution. The framework of the Bayesian network (BN) is then determined accordingly. In the case that the historical statistics of accidents are limited, a probabilistic estimation model that combines expert judgment and fuzzy set theory is established to determine the prior probabilities and the conditional probabilities of the BN nodes. Case studies of typical road tanker transportation accidents were carried out to show the risk level variation with both the internal and external conditions at different moments. Sensitivities of the parent nodes were analyzed, and the critical factors leading to accidents were identified. Studies show that this method can dynamically characterize the changes in both the probabilities and the consequence levels of road tanker transport accidents. Based on the vehicle's GPS data and the local environment, the proposed method can provide an estimation of the real-time risk for road tankers.

- **Keywords:** Road tanker; Real-time risk analysis; Bow-tie model; Bayesian network; Fuzzy set theory

Gui Fu, Xuecai Xie, Qingsong Jia, Zonghan Li, Ping Chen, Ying Ge. *The development history of accident causation models in the past 100 years: 24Model, a more modern accident causation model*. Pages 47-82.

Accident causation models mainly answer the following two questions: (i) why does an accident occur, and (ii) how does it occur? These models are the most important theoretical basis for safety science, and provide an important method for accident analysis and prevention. To understand accident causation models systematically and comprehensively, this work clarifies the development history of these models over the past 100 years. The work conducted in this study is summarised as follows: (i) The role and origin of accident causation models are introduced. (ii) A new method for classifying accident causation models is proposed. The method divides the accident causal models into linear and nonlinear accident causation models, and the latter are further divided into human-based, statistics-based, energy-based, and system-based accident models.

(iii) A review of 29 representative accident causation models proposed in the past 100 years is conducted. The theoretical basis, application flow, and application status of these models are highlighted. (iv) A detailed introduction to the 24Model, an accident causation model with theoretical innovation and more modern safety management, is presented. (v) A comparative analysis of various accident causation models and their development trends are discussed. (vi) This safety also summarises the application status of the accident causal model and prospects for future applications. The research findings of this study are as follows: (i) The newly proposed classification method of accident causation models clarifies the classification of accident causes. (ii) Each type of accident causation model has its own characteristics and application scope. In an accident analysis, an accident model that meets its industry characteristics should be selected. (iii) 'Organisational factors' will be replaced by more modern 'safety management systems', and people will pay more attention to the role of 'safety culture' in accident prevention. Accident causation models will develop in a linear and systematic way. (iv) The current accident causation models consist mainly of qualitative analysis and quantitative analysis, and will develop in the direction of dynamic analysis, accident prediction, and intelligent comprehensive analysis in the future.

- **Keywords:** Accident causation model; Development history; Accident analysis and prevention; 24Model; Model comparison analysis; Application status and prospect

Xin Wang, Yingjie Li, Wan Zhang, Jianli Zhao, Zeyan Wang. *Simultaneous SO2 and NO removal by pellets made of carbide slag and coal char in a bubbling fluidized-bed reactor*. Pages 83-94.

In this work, a simultaneous SO2/NO removal method using pellets made of carbide slag and coal char by extrusion-spheronization process was proposed. The effects of char type, reaction temperature, O2 concentration, initial NO/SO2 concentration and the addition of supporters on the simultaneous SO2/NO removal performance of the pellets made of carbide slag and coal char were investigated in a bubbling fluidized-bed reactor. CaO derived from carbide slag not only acts as an excellent desulfurizer but also catalyzes the reduction of NO by coal char. The results show that the pellets made of carbide slag and coal char possess better simultaneous SO2/NO removal performance than the pellets made of carbide slag and bio-char. The optimal reaction temperature range for SO2/NO removal by the pellets made of carbide slag and coal char is 850−875°C. The addition of the supporters such as Al2O3 and high alumina cement enhances the mechanical strength of the pellets. The pellets made of carbide slag and coal char seems promising for efficient simultaneous SO2/NO removal in the circulating fluidized bed decoupling combustion.

- **Keywords:** Carbide slag; Coal char; Pellets; Fluidization; Simultaneous SO2/NO removal

Rustam Abubakirov, Ming Yang, Nima Khakzad. *A risk-based approach to determination of optimal inspection intervals for buried oil pipelines*. Pages 95-107.

Corrosion is a significant concern causing tremendous losses to all pipeline operators. To combat this operational issue, new methods and tools are needed to analyze and model degradation, to predict failure, and finally to develop strategies for prevention, control, and mitigation of corrosion in pipelines. A practical inspection and maintenance program is crucial to prevent pipeline failures due to corrosion. Risk-based inspection (RBI) is an increasingly popular and trusted method to assess and develop inspection plans. However, the determination of optimal inspection intervals is still challenging in RBI. The present study aims to develop a dynamic Bayesian network (DBN)-based approach for optimization of inspection intervals. Based on inline inspection data and analytical

corrosion propagation models, DBN is applied for the estimation of both the internal and external corrosion damage as well as the probability of failure (PoF). The cost of failure (CoF) is estimated based on typical cost categories relevant to pipeline accidents. Risk is calculated as the product of PoF and CoF. A utility function to combine both the risk and the annual cost of the inspection program is also developed. The optimal interval can be found based on the curve of the utility function. The proposed approach is demonstrated through a real-world case study on an operating pipeline.

- **Keywords:** Pipeline; Corrosion; Inspection planning; Risk-based methodology

A.M. Birk, R. Eyssette, F. Heymes. *Analysis of BLEVE overpressure using spherical shock theory*. Pages 108-120.

The near-field hazards from BLEVE including blast, ground force, drag loading from the rapid liquid phase change and projectiles. There are several correlations available in the literature for the far field blast overpressure from a BLEVE, usually requiring the calculation of the available expansion energy and the application of correction factors. However, there is very little information available for near-field effects and how this is affected by the details of vessel failure. This work presents near-field blast overpressure data and prediction models to fill in this gap. First, experimental measurements of overpressure in the near-field of a small scale cylindrical controlled BLEVE experiments with propane (V=0.6L, d =50mm, L=300mm) were performed. Then, this work establishes a prediction model based solely on the vapour phase properties at failure, using shock tube overpressure prediction and spherical shock propagation models. The model predicts well the strongest tests and is conservative with all the others. Scaling the model up to larger scale experimental data from literature shows that it is transposable, proposing a simple physics-based prediction model for BLEVE overpressure.

- **Keywords:** BLEVE; Boiling liquid expanding vapor explosion; Explosion; Overpressure; Experimental results; Blast measurement; Lead shock; Prediction model; Modelling; Spherical shock

Tian Xie, Ruichao Wei, Zhi Wang, Jian Wang. *Comparative analysis of thermal oxidative decomposition and fire characteristics for different straw powders via thermogravimetry and cone calorimetry*. Pages 121-130.

Safety performance of straw powders, a primary component of biomass pellet fuel, remains challenging. In this work, three straw powders (soybean, peanut, and rape) were studied. Thermogravimetry and cone calorimetry were employed to investigate thermal oxidative decomposition characteristics and fire behaviors. Thermogravimetry (TG), micro-commercial thermogravimetry (DTG), and differential scanning calorimetry (DSC) curves showed that the thermal decomposition of the three samples proceeded in four stages. TG-DTG-DSC data also revealed that their ignition and burnout temperatures and mass loss rates were all distinct. Combustion indices of the three samples were ordered as RS>SS>PS. Based on the cone calorimetry results, critical heat fluxes for ignition were determined to be 25.31, 29.14, and 18.27kW/m2 for SS, PS, and RS, respectively. Critical fire properties such as ignition time, heat release rate intensity, and CO/CO2 ratio were influenced by biomass species and external heat fluxes. Compared with the other two samples, RS exhibited better burnout performance but was a greater fire hazard. Nevertheless, according to the hazard assessment, the three straw powder samples all had a high fire risk. Additional care must be taken in handling, storing, transporting, and utilizing straw powder in biomass pellet fuel processing.

- **Keywords:** Straw powders; Thermogravimetric analysis; Calorimetry; Thermal oxidative decomposition; Fire characteristics

Yong Sun, Jun He, Yunshan Wang, Gang Yang, Guangzhi Sun, Valérie Sage. *Experimental and CFD study of H2S oxidation by activated carbon prepared from cotton pulp black liquor*. Pages 131-139.

A porous activated carbon (AC) was synthesized from cotton black liquor, and the synthesis process was optimized using response surface method (RSM). The AC prepared under the optimal condition was applied to the direct H2S catalytic oxidation. Complete parametrical computational fluid-dynamic (CFD) model, coupling stoichiometric reaction with variation of porosity as the user-defined scalars (UDS), was developed to simulate the removal process. Various experiments, including breakthrough, pressure drops, and H2S conversion at different experimental conditions, were carried out. The CFD model was validated by results from the experiments, as the experiment results were found to adequately match model predictions. Hence, the model developed in this study can be a useful tool for studying the fluid dynamics of H2S oxidation by AC catalyst at investigated experimental conditions.

- **Keywords:** Activated carbon; Black liquor lignin, CFD; H2S

Eduarda Freitas Diogo Januário, Natália de Camargo Lima Beluci, Taynara Basso Vidovix, Marcelo Fernandes Vieira, Rosângela Bergamasco, Angélica Marquetotti Salcedo Vieira. *Functionalization of membrane surface by layer-by-layer self-assembly method for dyes removal*. Pages 140-148.

Membrane separation processes are an efficient method to manage the amount of wastewater improperly discharged into water due the use of dyes in industrial processes. Thus, polyethersulfone microfiltration membranes were modified with sulfuric acid, titanium dioxide (TiO2) and graphene oxide (GO) solutions by layer-by-layer self-assembly method via electrostatic interaction through a pressure-assisted filtration system. The characterization indicated that the proposed modification was successfully accomplished. The effect of TiO2 and GO masses deposited on the membrane surface was studied. MFTD1.0+GO2.5 membrane showed the best performance among synthesized series achieving a red bordeaux (BR) dye removal of 93.35 % and a flux recovery ratio of > 80 %. The treatment of dyes twilight yellow (TY) and safranin orange (SO) was investigated in this membrane achieving a rejection rate of 69.98 and 100 %, respectively. For dyes with high removal rates (BR and SO), other filtration cycles were performed and good results were accomplished. The proposed modification resulted in an efficient treatment of dyes with different characteristics as well as improvement of selectivity and antifouling properties of the membranes. Their reuse potential represents an additional environmental advantage of this process.

- **Keywords:** Polyethersulfone; Layer-by-layer; Dyes removal; Reuse; Antifouling; Wastewater

Tao Zeng, Guohua Chen, Yunfeng Yang, Peizhu Chen, Genserik Reniers. *Developing an advanced dynamic risk analysis method for fire-related domino effects*. Pages 149-160.

Domino effects are typically high impact low probability (HILP) accidents, whereby escalation effects triggered by fires are most frequent. The evolution of fire-related domino effects depends on synergistic effects and the performance of safety barriers, but those factors usually are time-dependent. In the present study, a methodology is developed to provide more accurate probabilities related to domino effects, by considering the temporal evolution of escalation vectors caused by time-dependent factors. The Dynamic Bayesian Network (DBN) approach is applied both to model the spatial-temporal propagation pattern of domino effects and to estimate the dynamic

probabilities of domino chains. The methodology is illustrated with a case study to determine the dynamic aspect of the probabilities of domino effects considering the impact of add-on (active and passive) safety barriers and taking into account synergistic effects. The critical units for facilitating domino propagation have been identified by the analysis of posterior probabilities, and further validated using graph theory. The methodology will be helpful for risk management and emergency decision-making of any chemical industrial area.

- **Keywords:** Domino effect; Dynamic Bayesian Network; Synergistic effect; Temporal evolution; Safety barrier

Youhei Nomura, Shuji Fukahori, Taku Fujiwara. *Removal of sulfamonomethoxine and its transformation byproducts from fresh aquaculture wastewater by a rotating advanced oxidation contactor equipped with zeolite/TiO2 composite sheets*. Pages 161-168.

A novel rotating advanced oxidation contactor (RAOC) equipped with high-silica zeolite/TiO2 composite sheets was applied to remove sulfamonomethoxine (SMM) and its transformation byproducts from fresh aquaculture wastewater (FAWW). Adsorption and photocatalysis of SMM was not interfered by coexisting substances in the FAWW. The combination of adsorption and photocatalysis by the RAOC degraded SMM more rapidly than photocatalysis alone, possibly because of the synergetic effect. Moreover, the increase in UV fluence rate (UVFR) enhanced SMM degradation, and the linear relationship between UVFR (0.9–3.6J/cm2/h) and the rate constant for SMM degradation was observed. The removal behavior of the transformation byproducts generated via hydroxylation of the aromatic ring of SMM was investigated, and their degradation was inhibited by the coexisting substances. The RAOC treatment was repeated five times without exchanging the composite sheets to evaluate the reusability of the composite sheet. The RAOC stably and completely eliminated SMM from the FAWW, showing the zeolite was regenerated by the photocatalysis of SMM adsorbed in the composite sheets. The results demonstrated that the RAOC effectively and stably removed SMM and its transformation byproducts from the FAWW.

- **Keywords:** Rotating advanced oxidation contactor; Zeolite/TiO2 composite sheet; Sulfamonomethoxine; Transformation byproducts; Fresh aquaculture wastewater

Reza Shokoohi, Nahid Ghobadi, Kazem Godini, Mahdi Hadi, Zeinab Atashzaban. *Antibiotic detection in a hospital wastewater and comparison of their removal rate by activated sludge and earthworm-based vermifilteration: Environmental risk assessment*. Pages 169-177.

The objective of the current research was to detect some antibiotics in hospital sewage and compare their removal rates reached using a vermifilter (VF) pilot and a real activated sludge (AS) treatment system. Six target antibiotics (ciprofloxacin, ofloxacin, sulfamethoxazole, trimethoprim, tetracycline and metronidazole) prescribed in the hospital were detected in the sewage and the removal rates via the two systems were examined. Three sampling points were chosen: the raw effluents from the hospital, VF and AS. Four sampling campaigns were performed over four months. Moreover, the environmental risk assessment was performed for all the antibiotics through estimating risk quotients (RQs). All the antibiotics were quantified in all the samples taken. It was found that ciprofloxacin had the highest concentration (7505.08–14731.88ng/L). The results revealed that the VF reactor had a better and more stable performance in removal of the antibiotics than the AS system even though all the antibiotics were present in the effluents of both the processes compared. Further, according to the calculated RQs, the hospital effluent had even high risk to algae and, generally, the VF system was capable of reducing the ecotoxicity of the antibiotics. Therefore, it could be confirmed that

earthworm-based vermifiltration can be considered as a promising alternative to conventional processes like AS, particularly when it comes to economic situations.

- **Keywords:** Ciprofloxacin; Conventional wastewater treatments; Eisenia fetida; Ecofilter; Ecotoxicity

Yan Cui, Noor Quddus, Chad V. Mashuga. *Bayesian network and game theory risk assessment model for third-party damage to oil and gas pipelines*. Pages 178-188.

Tremendous amounts of oil and gas products are transported in pipelines worldwide resulting in increasing interest to identify the hazards and evaluate the associated risks associated with this critical infrastructure. Third-party intrusion is one of the least quantifiable factors being considered during the pipeline hazard assessment stage despite the substantial contributing to the total number of oil and gas pipeline incidents. This is because a probabilistic risk assessment cannot reliably model human actions and be applied to intentional acts. Due to the distinctive motivations of third-party damage, an unintentional third-party damage Bayesian Network model and a game-theoretic model on malicious intrusion will therefore be built, to examine the mechanism of pipeline failure caused by this mode. This study is conducted aiming at investigating pipeline risk resulting from third-party damage, and will formulate risk assessment models to identify threats, prioritize risks and determine which integrity plan should apply to different pipeline segments given the condition of third-party interference (both the accidental damage and malicious acts).

- **Keywords:** Bayesian network; Game theory; Pipeline damage; Risk assessment; Pipeline safety; Pipeline hazard assessment

Song Sun, Mingyang Wang, Huadao Xing, Kanghua Gao, Yanyu Qiu. *A prediction model for debris scattering in vented gas deflagration*. Pages 189-196.

As one of the main modes of damage caused by gas explosions in industrial production, the debris generated by the explosion threatens the safety of surrounding personnel and buildings. By means of experimental research and theoretical modelling, the debris generated by the vented component was experimentally studied, and a predictive model of the scattering range of explosion-induced debris was proposed. Through experiments using a self-designed explosion test apparatus, it is found that the gas explosion exerts a quasi-static pressure, and the vented plate is cracked by the plastic hinge under deflagration load. According to the force and the motion equation of the debris, the predictive model of the debris trajectory was proposed by differentiating the scattering process. The distribution of random variables in the model was determined by experimental data, and the scattering range of explosive debris was obtained using the Monte Carlo method. By comparing the calculated results with experimental data gathered under three typical conditions, the model values were seen to agree with the experimental values, and this model can predict the scattering range of debris. The proposed prediction model for debris scattering can provide a reference for the design of works used to protect against debris damage and subsequent domino effect.

- **Keywords:** Gas vented explosion; Debris scattering; Monte Carlo method; Vented component

Hafida Lebik-Elhadi, Zacharias Frontistis, Hamid Ait-Amar, Farid Madjene, Dionissios Mantzavinos. *Degradation of pesticide thiamethoxam by heat – activated and ultrasound – activated persulfate:*

***Effect of key operating parameters and the water matrix*. Pages 197-207.**

This work studied the degradation of pesticide thiamethoxam (TMX) by heat-activated and ultrasound-activated persulfate systems. The effect of different parameters on degradation in ultrapure water, such as initial pH (3–10), sodium persulfate (SPS) concentration (50−1000mg/L), TMX concentration (1−10mg/L), temperature (20−70°C) and ultrasound power density (20−42W/L) were examined. For the heat-activated system, TMX degradation increased with increasing temperature and SPS concentration and was favored at pH 6; the activation energy was computed at 108.7kJ/mol based on the Arrhenius law. Ultrasound alone was capable of partially degrading TMX, but the process was favored in the presence of SPS. For the ultrasound-activated system, degradation increased with increasing SPS concentration and power density at pH 6. The effect of temperature was controversial since the beneficial effect of high temperatures on SPS activation is offset by the reduced sonochemical activity due to the "cushioning" effect. Regardless of the activation system, the presence of chloride, bicarbonate and humic acid impeded TMX removal. Besides, TMX degradation was reduced in actual matrices, i.e. wastewater and bottled water, showing the competition between TMX and other matrix constituents for free radicals. For either system, mineralization was slower than TMX degradation, implying the formation of persistent by-products.

- **Keywords:** Persulfate; Ultrasound; Heat; Mineralization; Water matrix; Synergy

Alexander Gorokhovsky, Maria Vikulova, Jose Ivan Escalante-Garcia, Elena Tretyachenko, Igor Burmistrov, Denis Kuznetsov, Diana Yuri. *Utilization of nickel-electroplating wastewaters in manufacturing of photocatalysts for water purification*. Pages 208-216.

A new route of purification/revalorization of nickel electroplating wastewaters is proposed. It is shown that chemical treatment of different nickel-electroplating wastewaters with aqueous dispersion of layered structure amorphous potassium polytitanate (PPT) successfully removed the nickel from the effluents. Moreover, the resulting solid products, obtained with optimal PPT doses, showed excellent and consistent photocatalytic properties in the visible range of solar radiation, which are independent on the characteristics of the wastewater i.e. pH, nickel contents or the presence of other heavy metals. On the other hand, after proper dilution, the resulting treated effluents can be returned to the municipal wastewater collectors. The mechanisms of the processes taking place during the treatment are analyzed.

- **Keywords:** Nickel electroplating; Wastewaters; Utilization; Photocatalyst; Water purification

Gang Fu, Juncheng Jiang, Lei Ni. *Research-scale three-phase jet foam generator design and foaming condition optimization based on Box–Behnken design*. Pages 217-225.

Three-phase foam, namely surfactant-particle stabilized foam is a promising material in pool fire extinguishment. However, its effectiveness has not been validated. In this study, a research-scale three-phase jet foam generator, which allowed adjustments of foam slurry composition, nozzle type, air flow rate and screen aperture, was developed. In order to optimize the foaming condition, a three-factor three-level Box–Behnken design (BBD) was adopted. Fly ash (FA) particles were used as the solid phase to generate three-phase foams. As a result, the FA supported foam exhibited better stability over conventional fire-fighting foam, especially when the particle concentration exceeded a threshold value. In addition, the BBD results presented a good agreement between experimental data and fitted models. The optimal foaming condition was determined by

numerical optimization. Small-scale fire extinguishing experiments were carried out and three-phase foam manifested better burnback performance compared to conventional fire-fighting foam. The design in this work can be used to study the firefighting efficiency of different three-phase foams and serve as a prototype to develop better generators for both lab research and practical application.

- **Keywords:** Three-phase foam; Fire extinguishing; Foam generator; Box–Behnken design; Optimization

Asif Matin, Umair Baig, M.A. Gondal. *Facile preparation of superwetting surfaces by dip-coating of silane for efficient separation of different types of oils from water*. Pages 226-238.

The application of membranes for environmental applications is becoming increasingly popular with researchers and scientists. This work reports the surface modification of membranes by a facile technique and its subsequent use for efficient separation of different types of oils from water. Stainless steel membranes were dip-coated with different concentrations of a low surface energy silane, perfluorooctyltrichlorosilane. The bonding between the silane film and substrate were confirmed by the use of spectroscopic techniques such as X-ray photoelectron spectroscopy and Fourier transform infrared spectroscopy. Scanning electron microscopic images showed the coatings to be continuous and uniform, an observation that was corroborated by the presence of almost spherical water droplets on different regions of the coated membrane. Contact angle measurements with representative oils and water revealed the superoleophilic (CA ~0°) and superhydrophobic (CA ~150.5°) character of the modified membrane after seven immersion cycles in the silane. The coated membrane was able to separate different types of oils from water with a high efficiency (>95 %) that was maintained after repeated passage. The separation mechanism was explained by a theoretical model that takes into account interfacial tension and pressure-driven forces. The usefulness of the coated membrane for large-scale applications was demonstrated by the high values of oil fluxes and the large intrusion pressures determined experimentally.

- **Keywords:** Membranes; Surface modification; Super wetting; Oil-water separation

Yixiang Zhang, Jianlu Zhu, Youmei Peng, Cunyong Song, Yuxing Li. *Experimental investigation of LNG release underwater and combustion behavior under crosswinds*. Pages 239-246.

Liquefied natural gas (LNG) trade has increased globally; therefore, assessments of the hazards of its accidental release and associated consequences must be conducted to ensure LNG security during marine transportation. This study aims to understand the dynamic behavior occurring when an LNG jet is released underwater and the combustion behavior of a flammable vapor cloud on the water's surface with airflows from 0 to 4m/s. A series of controlled LNG vertical jet release experiments were conducted using a cryogenic storage tank with three orifices. Various instruments were employed to measure the flow rate and pressure in pipelines during different leakage scenarios, and the emanating LNG vapor clouds were immediately ignited with the mass loss rate of 0.016, 0.037, and 0.049kg/s in three orifices, respectively. The flame behavior was recorded by a video camera. With respect to flame length rapidly decreased with crosswinds of 0−2m/s and then gradually decreased to a constant value with the velocities increase to 4m/s. A dimensionless number of Ri was employed to analyze the relative magnitude between the buoyancy force and transverse flow. The flame tilt angle was found in accordance trend with flame length for first increased and further reach to become constant at Ri−1 increase to 2. As existing correlations provide an overestimation, a new correlation was established to describe the flame length as a

function of crosswind speed, and a good prediction was found for measured tilt angles with the correlated values.

- **Keywords:** LNG leakage underwater; Flow rate and pressure; Flame length; Tilt angle; Crosswinds

Audrey Santandrea, Marine Gavard, Stéphanie Pacault, Alexis Vignes, Laurent Perrin, Olivier Dufaud. *'Knock on nanocellulose': Approaching the laminar burning velocity of powder-air flames*. Pages 247-259.

Due to their low sedimentation rate, nano-objects offer the opportunity to study flame propagation at low turbulence. The burning velocity was then estimated by flame visualization in two apparatuses: a vertical 1m long tube with a square cross-section and a 20L sphere equipped with visualization windows and a vent. This works aims to study the laminar burning velocity of nanocellulose by a direct visualization of the flame propagation within these devices. A high-speed video camera was used to record the flame propagation, and an estimation of the unstretched burning velocity was obtained through linear and nonlinear relationships relating the flame stretching and the flame velocities. Although these methods were initially established for gases, the organic nature of nanocellulose implies a fast devolatilization, which makes the application of the methods possible in this work. Similar results were obtained in both apparatuses in different turbulence conditions, proving the laminar burning velocity was approached. The laminar burning velocity for the nanocellulose was determined to be 21cms−1. This value, estimated through flame propagation visualization, was then compared to the value calculated by applying a semi-empiric correlation to the pressure-time evolution recorded during standard explosion tests in the 20L vessel.

- **Keywords:** Dust explosion; Nanocellulose; Flame propagation; Burning velocity; Nanopowder

Yeon-pyeong Jo, Yongheon Cho, Sungwon Hwang. *Dynamic analysis and optimization of flare network system for topside process of offshore plant*. Pages 260-269.

This study introduces a new approach for designing a flare network system that ensures economic feasibility and safety using dynamic simulation analysis with the gPROMS ProcessBuilder software. A case of "separator outlet blocked discharge" was selected as a pressure-relief scenario based on the American Petroleum Institute Standard 521, and design data from a previous offshore project were used. As the main process and flare network system were dynamically simulated, the effects of the pressure, temperature, and liquid-level changes in the vessel on the opening of the pressure safety valve (PSV) were analyzed. Then, dynamic simulation results, including those for the flare load, PSV back pressure, and Mach number, were compared with those obtained from a steady-state model employing the Aspen Flare System Analyzer. Lastly, the sizes of the PSVs, branch lines, and main headers were optimized to minimize the overall capital costs and ensure the safety of the flare network system. This methodology can be applied to all existing and newly designed flare network system to enhance safety and reduce capital costs.

- **Keywords:** Emergency flare emission; Dynamic simulation; Mach number calculation; Line sizing criteria; Pipe line optimization

Shang-Hao Liu, Bin Zhang, Chen-Rui Cao. *Assessing the thermal properties of [Bmim]NO3 through thermokinetic calculations and the energy equilibrium method*. Pages 270-276.

Using batteries to convert chemical energy into electrical energy is one of the significant technologies that must be enhanced in the 21st century. In the fuel battery development area, ionic liquids (ILs) are outstanding electrolytes for batteries. According to their thermophysical and phase equilibrium properties, ILs are widely used in different energy fields due to their diversity in the synthesis field. However, there are few detailed thermokinetic studies on ILs. To ensure the thermal safety of ILs in the process of creation, a commonly used IL, 1-butyl-3-methylimidazolium nitrate ([Bmim]NO3), was chosen for exploration. In this study, thermal decomposition characteristics were obtained by differential scanning calorimetry. The obtained data were input into the thermokinetic equation to determine the basic thermal hazards of [Bmim]NO3. In addition, based on thermal equilibrium theoretical models, the reaction kinetics and critical safety parameters were extrapolated for consideration. The influences of the sample mass and the overall heat transfer coefficient were simulated and discussed in 25.0g and 50.0g packages. The results showed that [Bmim]NO3 had a shorter TMRad and TCL (<1 day) when the temperature was greater than 200°C. Moreover, SADT<150°C can be used for evaluating the cooling system efficiency of [Bmim]NO3.

- **Keywords:** Ionic liquids; Heat transfer; Thermokinetic; Thermal hazard

Panteha Pirieh, Fereshteh Naeimpoor. *Multiple versus single response optimization in thiosulfate bio-removal and its products formation and function of optimum point in bioreactor*. Pages 277-291.

Sulfur oxidizing bacteria have been widely exploited to remove thiosulfate with adverse effects on human health and environment. Since formation of elemental sulfur among other thiosulfate oxidation products is advantageous in industrial applications, we tend to statistically screen (fractional factor design) and optimize (response surface methodology) the operating conditions in this study so that the final thiosulfate removal (Y1) and the highest sulfur production (Y2) become maximum along with the appropriate final sulfate formation (Y3). Optimum conditions were then examined in a stirred bioreactor. Screening results showed the definite effectiveness of six factors on all responses however level modification and optimization were necessary due to significant P-value of curvature. Single response optimizations (maximization of each response) resulted in dissimilar sets of optimal conditions. Multiple response (Y1 = 100 %, Y2 and Y3 = 50 %) optimization, using desirability function, was therefore used and resulted in agitation speed: 44 rpm, pH: 6.07, temperature: 24.7 °C, time: 2.64 day, inoculum ratio: 19.5 % and thiosulfate level: 2.87 mg l−1 as optimal conditions. Bioreactor experiments (agitation speeds: 30−90 rpm) under optimal conditions led to the highest S0 formation of 46 % and complete thiosulfate removal at 60 rpm and 40 h. Therefore, multiple response optimization followed by minor scale modifications can productively enhance industrial elemental sulfur formation from wastewater plants.

- **Keywords:** Thiosulfate bio-oxidation; Fractional factorial design; Multiple response optimization; Response surface methodology; Desirability function; Elemental sulfur

Mohammad Malakootian, Armita Shahesmaeili, Maryam Faraji, Hoda Amiri, Susana Silva Martinez. *Advanced oxidation processes for the removal of organophosphorus pesticides in aqueous matrices: A systematic review and meta-analysis*. Pages 292-307.

The advanced oxidation processes (AOPs), as an alternative technology to eliminate pesticides from aqueous environments, consist of several groups of technologies that have been used with high efficiency in the treatment of water and wastewater in recent decades. A systematic review of the scientific literature to evaluate the most common advanced oxidation processes (AOPs) for the removal of organophosphorus pesticides in

aqueous matrices is addressed in this study. Meta-analysis is also performed to provide a precise and robust summary estimate after a systematic and rigorous integration of the available evidence. In the current study, 9 sub-groups of AOPs were reviewed, such as electrochemical, UV/H2O2 photolysis, photocatalysis, Fenton-type, plasma, gamma irradiation, sulfate-based catalyst, sonolysis and ozonation technology for organophosphorus pesticides degradation. The random effects model was used to estimate the pooled measurements and 95 % confidence intervals (95 % CI). In total, six studies were included in this review. All studies, except one, used the photocatalytic process as AOP. The average pooled percentage of AOP for pesticide degradation was 66.8 (95 % CI: 58.1–75.6). In addition, the most studied pesticides are chlorpyrifos and diazinon which, according to the results of the meta-analysis, the photocatalytic process has the highest efficiency of diazinon elimination with an average percentage of 79.2 (95 % CI: 76.8–81.5).

- **Keywords:** AOPs; Degradation; Meta-analysis; Pesticides; Remediation; Statistics analysis

Yizhi Hong, Hans J. Pasman, Noor Quddus, M. Sam Mannan. *Supporting risk management decision making by converting linguistic graded qualitative risk matrices through interval type-2 fuzzy sets*. Pages 308-322.

Risk matrices are widely used to present results of qualitative and semi-quantitative risk assessment for risk management decision making. There are different types of risk matrix category definitions according to the function and risk acceptance criteria. This paper reviews some general weaknesses of current risk matrices and proposes a method to improve the reading ambiguity of linguistically graded qualitative risk matrices. Main topic of this paper is the type of risk matrix that grades event consequence and frequency categories in linguistic terms. Because different people understand the meaning of these terms differently, the aim is to convert subjective quantified term inputs produced by a number of experts independently as much as possible to objective values creating at the same time a clearer and more discriminative result. In other words, the method involves asking various expert users independently to estimate numerical intervals of linguistic grades of event consequence and frequency on a continuous scale while maintaining risk acceptance levels. It is applying a second-generation fuzzy logic technique to express linguistic terms in numbers, called computing with words. This interval type-2 fuzzy system has evolved lately as a decision-making support tool and appears to be well suited to handle uncertainty intrinsic to qualitative linguistic grades, fusing different individual expert estimates in an objective way and to facilitate the reading resolution by introducing gliding numerical scales instead of discrete categories. Examples are given to illustrate the method as well as the use of the technique to aggregate a number of different qualitative risk matrix types into one unified risk matrix. The latter is useful in case a corporate-wide risk matrix exists to standardize risk management across the company, but older versions may still be around which should be fused with the newer ones.

- **Keywords:** Risk matrix; Interval type-2 fuzzy set; Linguistic grades; Risk management

S. Abbasi, M. Mirghorayshi, S. Zinadini, A.A. Zinatizadeh. *A novel single continuous electrocoagulation process for treatment of licorice processing wastewater: Optimization of operating factors using RSM*. Pages 323-332.

The potential application of a novel continuous electrocoagulation (EC) reactor for simultaneous removal of color, chemical oxygen demand (COD), turbidity, and alkalinity

from a real licorice processing wastewater was investigated. The individual and interactive effects of four key independent variables (electrolysis time, current density, NaCl concentration, and mixing intensity) was evaluated. The results suggested that color and COD removal enhances with increasing electrolysis time, current density, and mixing intensity and remains practically constant by adding higher concentrations of NaCl. The application of continuous EC process under optimal conditions, such as: electrolysis time (81.8min), current density (350 A/m2), NaCl concentration (300mg/L), mixing intensity (45rpm) allows to achieve these promised removal efficiencies: 90.1 % color, 89.4 % COD, 82 % turbidity, and 73.3 % alkalinity.

- **Keywords:** Licorice processing wastewater; Electrocoagulation process; Iron electrodes; Continuous operating mode; Central composite design (CCD); Response surface methodology (RSM)

Pablo Marín, Aurelio Vega, Fernando V. Díez, Salvador Ordóñez. *Control of regenerative catalytic oxidizers used in coal mine ventilation air methane exploitation*. Pages 333-342.

Ventilation air methane in coal mining has an important environmental impact, since methane is a strong greenhouse gas (1kg of methane is equivalent to 28kg of carbon dioxide). The oxidation of methane in regenerative oxidizers can be an attractive technique to exploit this resource. Thus, part of the heat released by the reaction can potentially be recovered, in addition to decreasing methane environmental impact. However, the concentration of methane in the mine ventilation air may change considerably with respect to the oxidizer design value, which have negative consequences. An increase in concentration can produce overheating (with possible damage to the unit), while a decrease in concentration may cause the extinction of the reaction. In this work, three control systems have been considered in order to deal with these issues: proportional-integral-derivative (PID) and proportional-integral (PI) feedback controllers, and model predictive controller (MPC). The control action is based on regulating the heat extracted from the oxidizer by adjusting a hot gas purge from the centre of the reactor. First, the control systems have been designed (i.e. the tuning parameters of the controller have been calculated). To carry out the design of the controllers, a simplified dynamic model was obtained from a complex model of the oxidizer. Then, the performance of the controlled oxidizer has been simulated for different types of disturbances. In these simulations, the simple PID controller performed well, and the MPC exhibited the fastest response.

- **Keywords:** Dynamic reactor; Periodic operation; Reverse flow reactor; Methane emissions; Reactor modelling

Xiaozhe Yu, Jianliang Yu, Xinyan Zhang, Wentao Ji, Xianshu Lv, Yujie Hou, Zhiyong Li, Xingqing Yan. *Combustion behaviors and residues characteristics in hydrogen/aluminum dust hybrid explosions*. Pages 343-352.

Hybrid explosion experiments of hydrogen/aluminum dust in open space were performed. Aluminum dust with a median diameter of 56.18μm was mixed with hydrogen at different volume concentrations (0 %, 5 % and 10 %). Flame propagation was recorded by a high-speed camera. The explosion residues were observed by a scanning electron microscope, and their compositions were analyzed by X-ray photoelectron spectroscopy. The flame propagation velocities and structures, explosion residues and the combustion reaction mechanisms of hydrogen/aluminum dust mixtures were elucidated. The results show that the addition of hydrogen can increase the flame brightness and improve the continuity of the flame front. In the flame propagation process of a hydrogen/aluminum dust hybrid explosion, a micro-diffusion flame and asymmetric flame appeared

simultaneously. Compared with pure aluminum dust combustion in air, when 5 % hydrogen-air mixtures were used to disperse the dust, the flame propagation velocities decreased by 0.11-0.15m/s. Attributable to a variety of intermediate products competing for oxygen and absorbing heat, the hybrid explosion residues cooled faster, porous oxide layers and incompletely oxidized aluminum spheres with small particle sizes were formed. The XPS showed that Al2O3, Al(OH)3, AlO(OH) and other complex products appeared in the combustion reactions. On this basis, a combustion model of hydrogen/aluminum dust hybrid explosion was established.

- **Keywords:** Hybrid explosion; Hydrogen/aluminum dust; Flame propagation; Explosion residues

Jian Zhang, Jingyu An, Zhihui Wen, Kaixuan Zhang, Rongkun Pan, Nahid Akter Al Mamun. *Numerical investigation of coal self-heating in longwall goaf considering airflow leakage from mining induced crack*. Pages 353-370.

Self-heating of coal is a long-standing hazard and pollution source in longwall goaf and abnormal air leakage into goaf is a key yet complex drive to the hazard. To investigate such a problem with more insights, a numerical model without considering coal moisture is established based on a Shendong longwall. Abnormal air leakage into goaf mainly sources from the edge cracks resulting in presence of high level oxygen (8 %~13 %) in start-off area of the longwall. Two heating liable regimes were identified: one is behind longwall face and another one locates in the start-off zone. Heating in the start-off zone develops more quickly than that in heating regime one. On day 25 the maximum temperature of regime two can rise to 500K while it can only increase to approximately 340K in regime one. The heating spot behind longwall face tends to be self-suppressed with longwall advancing while the heating in the start-off zone can develop to a spontaneous combustion incident due to constant airflow leakage from the mining induced cracks. A wide range of inertisation plans including different locations, strategies, and flowrates of nitrogen injection were conducted. An optimum inertisation plan is to proactively inject inert gas with a low flowrate (e.g. 122m3/h) from a seal along the start-off line. A high flowrate of nitrogen stream is preferable to suppress an on-going heating and the reactive inertisation should be maintained for a long run otherwise the heating is very likely to re-develop.

- **Keywords:** Self-heating of coal; Airflow leakage; Mining-induced crack; Numerical simulation; Goaf inertisation

Agnès Grandjean, Yves Barré, Audrey Hertz, Virginie Fremy, Jérémy Mascarade, Eric Louradour, Thierry Prevost. *Comparing hexacyanoferrate loaded onto silica, silicotitanate and chabazite sorbents for Cs extraction with a continuous-flow fixed-bed setup: Methods and pitfalls*. Pages 371-380.

Radioactive 137Cs is one of the most common and problematic radionuclides in nuclear wastes. Decontamination typically involves passing the waste in continuous flow through an agitated or fixed bed reactor containing an efficient sorbent. There are many articles in the literature describing a broad spectrum of highly efficient sorbents. However,their properties is often difficult, mainly because the experimental conditions used differ. We describe the series of experiments that need to be performed to characterize Cs sorbents and illustrate by comparing three of these that, for the extraction of trace elements, the kinetics and selectivity of the exchange process are far more important than the maximum extraction capacity of the material.

- **Keywords:** Water treatment; Cs; Fixed bed process; Hexacyanoferrate; Zeolite; Silicotitanate

Jasir Jawad, Rafael de Pelegrini Soares, Luc N. Véchot, Marcelo Castier. *Dynamics of gas flow between interconnected vessels: Experiments and simulations*. Pages 381-391.

The emergency relief systems of pressure vessels often direct their discharge to containment vessels known as catch tanks or dump tanks, which are part of effluent handling systems. Although many models exists for vent sizing and critical flow calculation, there is less information about the impact of depressurization on the catch tank. This work addresses this topic by presenting experimental and simulation studies. We report experimental temperatures and pressures in the pressurized vessel and in the catch tank during the depressurization of air or helium from several initial conditions. A reproducibility study demonstrates the excellent agreement among the results of different experimental runs. On simulation, we present results of the depressurization of a vessel connected to a catch tank. To accomplish this, an existing dynamic simulator is extended by including a one-dimensional transient heat transfer model and by enabling the simulation of interconnected vessels. The experimental and calculated pressure profiles are generally in very good agreement. The agreement of the experimental and calculated temperature profiles is good but the calculated profiles tend to overestimate the temperature variations in each vessel during the depressurization process compared to the experimental data.

- **Keywords:** Depressurization; Catch tank; Phase equilibrium; Equation of state; Dynamic simulation

Chao Chen, Genserik Reniers, Nima Khakzad. *Cost-benefit management of intentional domino effects in chemical industrial areas*. Pages 392-405.

Chemical industrial areas comprising various hazardous installations may be attacked by adversaries, triggering possible intentional domino effects. Compared with accidental domino effects, intentional domino effects may be more difficult to prevent since intelligent and strategic adversaries can adapt their tactics according to protection measures. However, how and to what extent domino effects affect security management is ignored in previous studies. This study proposes a methodology to prevent and mitigate intentional domino effects taking into consideration economic issues in the decision-making process on safety and security resources. The methodology is divided into five parts: threat analysis, vulnerability analysis of installations with respect to intentional attacks, vulnerability analysis of installations subject to possible domino effects caused by the attacks, cost-benefit analysis, and optimization. Net present value of benefits (NPVB) is employed and quantified in the cost-benefit analysis to determine whether a protection strategy (a combination of safety and security measures) is profitable, or not. Besides, an optimization algorithm called "PROTOPT" based on "maximin" strategy is developed to achieve the most profitable protection strategy. An illustrated case study shows that domino effects can not be ignored in security management since they may have a profound impact on adversaries' strategies.

- **Keywords:** Intentional domino effects; Vulnerability assessment; Cost-benefit analysis; Dynamic graphs; Safety and security measures; Optimization

Agostina Chiavola, Camilla Di Marcantonio, Maria Rosaria Boni, Stefano Biagioli, Alessandro Frugis, Giancarlo Cecchini. *Experimental investigation on the perfluorooctanoic and perfluorooctane sulfonic acids fate and behaviour in the activated sludge reactor*. Pages 406-415.

Perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) are the most investigated compounds in the class of perfluoroalkyl substances for their persistence and wider diffusion in the environment. However, fate and behaviour of PFOA and PFOS in the Wastewater Treatment Plants (WWTPs) have not been fully understood yet. The aim of the present study was to obtain a better understanding of the processes occurring to PFOS and PFOA in the activated sludge reactor. Several experimental tests were performed in the presence of activated sludge and sterilized sludge. PFOA and PFOS showed removals from the liquid phase from 59 % to 68 % and from 66 % to 96 %, respectively, for initial concentrations from 200ng/L to 4000ng/L in the presence of activated sludge. A significant fraction of the initial contaminant load was found adsorbed on the sludge, mainly in the case of PFOS. Other processes occurred, not fully identified, which were responsible of a further loss from the system. Leaching tests showed negligible release of the adsorbed pollutants from the sludge. Carbon and ammonia removal in the activated sludge reactor were not significantly affected by the presence of PFOA and PFOS. The pseudo-second order kinetic model and the Freundlich isotherm provided the best fitting of the experimental data.

- **Keywords:** Activated sludge; Adsorption; Inhibition effect; Perfluorooctane sulfonic acid; Perfluorooctanoic acid; Respirometric test

Kun Hu, Guohua Chen, Rouzbeh Abbassi, Zhihang Zhou, Tao Zeng, Yi Yang. *A novel approach to distinguish the uniform and non-uniform distribution of blast loads in process industry*. Pages 416-428.

The blast load distribution is an important factor affecting the accuracy of structural damage and domino effect analysis caused by explosions in petroleum and chemical industries. The distribution is usually treated as the uniform or non-uniform and the latter is more suitable for the real scenarios. However, the applicability of the uniform distribution has not been studied in details. In the present study, both the blast load intensity model (BLIM) and blast damage intensity model (BDIM) are developed to represent uniform or non-uniform blast loads quantitatively. Three explosion types (free air burst, air burst and surface burst) and three target structural surfaces (rectangular plates, cylindrical shells and spherical shells) are considered in BLIM and BDIM. The element superposition method based on finite element model (FEM) is proposed, which can solve BLIM and BDIM accurately. Furthermore, the relative difference between the uniform and non-uniform distribution can be obtained on basis of BLIM and BDIM. Finally, the application condition for the rectangular plates - critical stand-off distances with the relative difference of 5%, is defined and verified to distinguish the uniform and non-uniform distribution. The study can provide an insight into the proper application of blast load distribution.

- **Keywords:** Blast load distribution; Blast load intensity model (BLIM); Blast damage intensity model (BLDIM); Element superposition method; Critical stand-off distances

Xianzhao Song, Hao Su, Lifeng Xie, Bin Li, Yong Cao, Yongxu Wang. *Experimental investigations of the ignition delay time, initial ignition energy and lower explosion limit of zirconium powder clouds in a 20L cylindrical vessel*. Pages 429-439.

Zirconium powder, a main potential dangerous source in nuclear industry, has been focused on its explosion characteristics in this paper. Experiments were performed in a 20 L cylindrical explosion vessel with the influences of initial ignition energy, ignition delay time and zirconium concentration. Results showed that the maximum explosion pressure of zirconium-air mixture rose with the increase of the initial ignition energy, and a peak value was obtained with the variation of the ignition delay time. Lower explosion

limit with the initial ignition energy of 10 kJ is 10 g/m³. Furthermore, explosion severity parameters, including maximum explosion pressure, maximum rate of pressure rise and maximum explosion index of zirconium-air mixture, were also obtained with the coupling variation between initial ignition energy and dust concentration. Research results and data obtained are a supplement to the utilization and safety operation of zirconium powders.

- **Keywords:** Zirconium powder; Dust-dispersion time; Maximum explosion pressure; Maximum rate of pressure rise; Explosion index; Concentration

Mohamadreza Massoudinejad, Saeed Motesaddi Zarandi, Mostafa M Amini, Seyed Mohsen Mohseni. *Enhancing photo-precipitation of chromate with carboxyl radicals: Kinetic, energy analysis and sludge survey*. Pages 440-447.

This study aims to develop a process based on the UV irradiation of TiO2 and carboxyl anion (UTC) to create reducer agents for photo-precipitation of the chromate. To perform the RSM-based optimization, a central composite design (CCD) function was employed for modeling and optimization. Based on this model, the stationary points for catalyst dosage, formate dosage, initial CrVI concentration and time were 5.34mgL−1, 3.34mgL−1, 123.15mgL−1, and 6.99 min, respectively. Moreover, the maximum reduction performance was reached as 98.44 and 97.22% at the modeling and experimental conditions. Therefore, the weight ratio of 5:2:120 (TiO2: FM: Cr), with 82.4% reduction of Cr and without formate remaining was chosen as the optimal and practical point. Nature of the Cr and the type of sludge created at different weight ratio in UTC process recognizable with different colors and FTIR spectra. The red and green color in sludge are due to the presence of CrO3 and Cr(OH)3 respectively, and the brown or black sludge are due to the presence of both Substances. Finally, the computational results shown with concentration increased from 33.75 to 120mgL−1 rate constant (kobs) decreases from 0.4257 to 0.1313min−1 while photoreaction rate (robs) increases from 14.36 to 15.75mgL−1min−1. Also, during Cr concentration increased from 33.75 to 120, electrical energy per order increase from 2.29 to 7.16 to 7.47–9.84 kwh.m-3.

- **Keywords:** Chromate; Formate; Reduction; Energy consumption; Kinetic; Sludge