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Yanhua Xie, Lulu Ren, Xueqian Zhu, Xi Gou, Siyu Chen. *Physical and chemical treatments for removal of perchlorate from water–A review*. Pages 180-198.

Perchlorate, which could not be easily degraded in the environment, is a persistent inorganic pollutant in water with high water-solubility, diffusivity, and stability. Its pollution has become a global environmental problem. Perchlorate in surface water and groundwater can keep in food and drinking water by various ways, which may cause a series of healthy problems in human body. Physical and chemical treatments are the technologies commonly used to remove perchlorate from water. This review begins with the existing treatments of perchlorate in water, then describes the perchlorate pollution status in different countries and its hazard for human being. In addition, the key findings of technologies and materials of physical and chemical treatments on perchlorate removal from water up to now are systematically summarized, and also the following research findings in recent years are elaborated in detail, such as the key findings, mechanisms, influencing factors, advantages and disadvantages. In particular, a novel material of nanoscale zero-valent iron (nZVI) which is used to remove perchlorate, is also presented. The coated nZVI introduced in this paper is superior for treating high-concentration perchlorate. This overall summary of the technologies and materials currently used can guide future studies on the removal of perchlorate from water.

- **Keywords:** Perchlorate removal; Water; Physical-chemical treatment; Chemical treatment; Nanoscale zero-valent iron (nZVI)

Sunil S. Suresh, Sateesh Bonda, Smita Mohanty, Sanjay K. Nayak. *A review on computer waste with its special insight to toxic elements, segregation and recycling techniques*. Pages 477-493.

Being a significant part of waste electrical and electronic equipment (WEEE), computer waste is gaining more attention due to its tremendous generation and toxic environmental concerns. The complex and diverse material content in the computer makes them ideal for recycling. At the same time, presence of hazardous contents such as flame retardants and heavy metals makes obstructions in recycling procedure. An enormous amount of computer wastes are either landfilled or incinerated, which results in leaching of chemicals and emission of toxic gases respectively. This paper reviews the information related to the role of computers in WEEE stream, hazardous components in computer waste stream, possibilities of segregation and the recycling of different components of the computer waste. A methodological segregation and recycling of the

computer waste components is more economical as compared to landfilling and incineration. Ultimately, natural petroleum resources can be conserved by recycling waste products which leads to the sustainable development of novel products. Furthermore, this review is helpful to sustainable development, in recycling procedure product formulation from computer waste products.

- **Keywords:** WEEE; Computer waste management; Hazardous; Recycling; Flame retardants

Mostafa Hossein Beyki, Javad Malakootikhah, Farzaneh Shemirani, Sara Minaeian. *Magnetic CoFe2O4@ melamine based hyper-crosslinked polymer: A multivalent dendronized nanostructure for fast bacteria capturing from real samples*. Pages 14-21.

Polymeric compounds are main types of advanced materials to prepare antibacterial coating as well as water treatment system hence this work was aimed to prepare a polymeric nanostructure with excellent bacteria capture efficiency. Dendronized melamine – resorcinol was synthesized by a condensation reaction. To simplify polymer collection from aqueous solutions, a magnetic nanocomposite of the polymer was also prepared. For this purpose, CoFe2O4 nanoparticles were synthesized by solid-state combustion route using cellulose as fuel. Bacteria removal efficiency was studied by uptake of Gram-negative (Escherichia coli) and Gram-positive (Bacillus subtilis) bacteria from water, milk and fruit juice samples. Effective parameter on the capturing efficiency including; solution pH, contact time and nanocomposite dosage were optimized. Results confirmed the positive role of presented nanostructure for fast capturing of bacterial pathogens with high efficiency (more than 99%).

- **Keywords:** Antimicrobial; Escherichia coli; Bacillus subtilis; CoFe2O4; Dendronized polymer; Food safety

Debarati Mukherjee, Priyankari Bhattacharya, Animesh Jana, Sandipan Bhattacharya, Subhendu Sarkar, Sourja Ghosh, Swachchha Majumdar, Snehasikta Swarnakar. *Synthesis of ceramic ultrafiltration membrane and application in membrane bioreactor process for pesticide remediation from wastewater*. Pages 22-33.

The efficiency of membrane bioreactor (MBR) process involving indigenously developed ceramic membranes was explored for management of wastewater containing toxic pesticides like atrazine. Performance of the MBR process was compared for clay-alumina based ceramic microfiltration membranes (MF-MBR) with that of an indigenously developed new ceramic ultrafiltration membrane (UF-MBR). The UF membrane was prepared on the macroporous support tubes using iron oxide nanoparticles synthesized by green route from Aloe vera leaf extract, with chitosan as matrix and glutaraldehyde as cross-linker. The synthesized membrane was characterized in terms of X-ray diffraction, field emission scanning electron microscopy, Fourier transform infrared spectroscopy, pore diameter and molecular weight cut off, etc. Microorganisms isolated from activated sludge of a pilot scale MBR plant were optimized to enhance the biodegradation efficiency of atrazine. Compared to the MF-MBR process, the UF-MBR process showed about 15% increase in atrazine removal, lower membrane fouling and complete separation of the biomass in the synthetic system. Performance of the UF-MBR process was further analyzed with domestic and industrial wastewater simulated with atrazine. In addition, toxicity assay of the UF-MBR treated water was performed on an aquatic model, Radix balthica indicating that the permeate could be safely disposed into the environment.

- **Keywords:** Ceramic ultrafiltration membrane; Green synthesized iron oxide nanoparticles; Membrane bioreactor (MBR); Atrazine; Toxicity assay

P.I. Omwene, M. Kobya. *Treatment of domestic wastewater phosphate by electrocoagulation using Fe and Al electrodes: A comparative study*. Pages 34-51.

In this work, phosphorus removal from domestic wastewater was studied through electrocoagulation (EC) using iron (Fe) and aluminium (Al) anodes in a batch EC reactor. Key parameters investigated include; initial pH, initial phosphorus concentration (Ci), reaction time, current density (j), metal-to-phosphorous ratio, charge loading (q) and electrode type. The Al/P mole ratio at current densities of 10, 20, 30 and 40A/m2 was obtained as 0.84, 1.68, 0.95 and 0.77, respectively, while the Fe/P mole ratio for these current densities was calculated as 1.81, 3.29, 4.09 and 4.48, respectively. The optimums to obtain <0.01mg/L effluent P concentration at Ci=52mg/L PO4-P were; pHi=4, j=20A/m2 and EC time=100min (q=954C) for Fe electrode, whereas for Al electrode, the optimums were; EC time=50min (q=372C), pHi=4, j=20A/m2. Also, the final pHf increased with increase in EC time; when pHi=4,Ci=52mg/L and j=20A/m2, the final pHf was 8.52 at 50min for Al electrode and 10.62 at 100min for Fe electrode. The operating costs, energy and electrode consumptions were calculated as 1.032$/m3, 1.143kWh/m3 and 0.218kg/m3 respectively for Al electrode and 1.343$/m3, 4.179kWh/m3 and 0.884kg/m3, respectively for Fe electrodes. Overall, Al anodes provided a higher phosphorus removal efficiency in a shorter EC time and lesser metal-to-phosphorous ratio compared to Fe anodes.

- **Keywords:** Phosphorus removal; Electrocoagulation; Domestic wastewater; Al and Fe electrodes

Qingwei Guan, Wentao Ji, Xingqing Yan, Jianliang Yu, Futong Yao, Dong Zhang. *Effect of fully blocked non-rigid boundary conditions on detonation wave*. Pages 52-60.

For the past half century, the research on boundary conditions on the detonation wave resulting in a velocity deficit or detonation failure mainly focused on the rough-walled or acoustically absorbing condition in one/two-dimensional models. In this paper, experiments on gaseous detonation propagation are conducted in the tube fully blocked by the non-rigid obstacles, under 20kPa with the explosive gas of C2H2+2.5O2+nAr. The polypropylene membrane (PET) is selected as the non-rigid obstacle in this paper. The detonation wave behavior is to decelerate, accelerate, and overdrive prior to reaching a stable state once passing through the PET obstacles. When the initial pressure decreases or the layers of PET obstacle increases, the detonation wave will transit from a velocity deficit mode to a failure mode after deceleration occurs. With the PET layers increasing, the velocity minimum decreases continuously from 0.61vCJ (m=1) to 0.23vCJ (m=8). The propagation mode is associated with the average diameter of the hole after passing through the PET obstacles. The detonation wave will diffract when the average diameter decreases. In addition, the Mach reflection degenerates to the expansion wave and self-ignition ceases. As the shock is reflected from the tube wall, the initial regular reflection changes to a Mach reflection and auto-ignition forms again. For the multi-PET obstacles, the velocity after obstacles fluctuates more violently. The instability is regarded as the critical factor in the deceleration and acceleration.

- **Keywords:** Gaseous detonation; Non-rigid boundary conditions; Velocity deficit; Detonation failure

Bahman Ramavandi, Ghorban Asgari. *Comparative study of sun-dried and oven-dried Malva sylvestris biomass for high-rate Cu(II) removal from wastewater*. Pages 61-73.

This study compared the sun- and oven-dried powdered Malva sylvestris for removing Cu(II) from aqueous solution. The fresh and Cu-loaded adsorbents characteristics were analyzed by Fourier transform infrared spectroscopy, Brunauer–Emmett–Teller testing and scanning electron microscopy. The studied parameters that affect adsorption capacity were pH (2–7), initial copper concentration (50–150mg/L), contact time (3–60min), adsorbent dosage (1–20g/L) and temperature (10–35°C). The results showed that the maximum removal of Cu(II) was observed at pH 5 for both adsorbents. The amount of Cu(II) adsorbed onto both adsorbents increased as the contact time and the initial concentration of Cu(II) increased. The adsorbents exhibited the highest Cu(II) removal at a temperature of 35°C. The adsorption data obtained at different temperatures was described well by the Langmuir isotherm (qm=172.61–202.81mg/g for oven-dried and 118.49–133.45mg/g for sun-dried) and the pseudo second-order kinetic model (R2=0.999 and 0.993–0.997 for oven- and sun-dried, respectively). An electroplating wastewater sample was effectively treated using oven-dried powdered M. sylvestris. The adsorption efficiency of the oven- and sun-dried M. sylvestris after five reuses was 70.4% and 26.1%, respectively. Generally, the oven-dried adsorbent was shown to be more effective than the sun-dried for removal of Cu(II) from wastewater. The cost assessment indicated that the oven-dried M. sylvestris is a more economical adsorbent than sun-dried one.

- **Keywords:** Adsorption; Cu(II); Electroplating wastewater; Malva sylvestris; Sun-dried; Oven-dried

Anshu Priya, Subrata Hait. *Toxicity characterization of metals from various waste printed circuit boards*. Pages 74-81.

Toxicity characterization (TC) of printed circuit board (PCB) of various obsolete electrical and electronic equipment (EEE) was performed. The end-of-life EEE considered in the study include personal computer (PC), laptop, washing machine (WM), television (TV) and air conditioner (AC). The standardized procedures i.e. EP, TCLP, ASTM Method D-3987 and SPLP were employed for toxicity characterization of PCBs in terms of metal leachability against their total metallic contents. Further, the standard SPLP was modified (MSPLP) to imitate Indian acid rain conditions to comparatively assess metal leachability. Except Se, there was statistically significant ($P<0.05$) difference in metal contents of PCBs from different sources with Cu (maximum: 231133±3889mg/kg in laptop) and Pb (maximum: 73900±22100mg/kg in laptop) being the predominant metallic species. The TC test conditions showed statistically significant ($P<0.05$) difference in metal leachability from respective EEE. Results indicated that Pb (maximum: 226.74±3.11mg/l in TCLP for laptop) and Ni (maximum: 0.942±0.053mg/l in SPLP for AC) in leachates exceeded the threshold toxicity limit. The general sequence of metal leachability, from most labile to least labile, from waste PCBs was: Pb>Cu>Zn>Al>Ni>Cd>Se>As>Ba. Except Pb, Cu and Zn, the ASTM procedure at neutral pH showed insignificant metal leachability. Standard SPLP and the MSPLP showed similar effect of Indian and western acid rain conditions on metal leachability. Greater leachability of Pb and Ni simultaneously indicated possible risk to the environment upon e-waste disposal.

- **Keywords:** E-waste; Printed circuit board; Metals; Leaching; Toxicity characterization; Hazardous waste

Niloofar Abedinzadeh, Mahmood Shariat, Sayed Masoud Monavari, Alireza Pendashteh. *Evaluation of color and COD removal by Fenton from biologically (SBR) pre-treated pulp and paper wastewater*. Pages 82-91.

Pulp and paper industry has generated a higher contamination burden of the final mill wastewater which must be further treated to comply with the standards imposed by the legislation requirement. In this study, the removal efficiencies for chemical oxygen demand (COD) and color from pulp and paper wastewater using sequencing batch

reactor (SBR) in combination with advanced oxidation processes (AOPs) at a bench scale were investigated. Response surface methodology (RSM) based on a three-variable-three-level central composite design (CCD) was employed to optimize the SBR process. At the optimal conditions of initial COD of 1000mg/L, MLSS of 3000mg/L and cycle time of 24h, 74.8% COD, 58.3% of color removal and 80mL/g of SVI were obtained in the pretreatment stage. The use of Fenton oxidation as post-treatment enhanced COD reduction and color removal. A percentage of 92.1% COD reduction and 90.3% of color removal was achieved in dosages of 3mM Fe2+ and 9mM H2O2 at pH of 3.0 for a reaction time of 30min, while a total of 98% reduction of COD and 94% removal of color for the combined treatment was achieved.

- **Keywords:** Pulp and paper wastewater; SBR; Fenton; RSM

Prerna Jain, William J. Rogers, Hans J. Pasman, Kelly K. Keim, M. Sam Mannan. *A Resilience-based Integrated Process Systems Hazard Analysis (RIPSHA) approach: Part I plant system layer*. Pages 92-105.

In recent years, the chemical process industry has witnessed increased process safety management challenges. One of the initial steps in process safety and risk management of any facility is hazard identification and analysis. Two types of factors: 1) technical (e.g., equipment malfunction), and 2) social (e.g., human and organizational factors) are important in analyzing hazards of a socio-technical process system as a whole. With the conventional process hazard analysis (PHA) methods, there is a tendency to overlook the potential impact of socio-technical systems on the health and sustainment of safeguards. This disregard leads to ignoring social factors, such as shift handover communication, downtime, operating and maintenance procedures, and more. This need calls for the development of a holistic and integrated systems framework for hazard analysis. This paper presents a novel hazards analysis approach that incorporates both technical and social factors within a single analysis method called Resilience-based Integrated Process Systems Hazard Analysis (RIPSHA). This approach is based on the following resilience aspects – 'early detection', 'error tolerant design', 'plasticity', and 'recoverability'. This work establishes and presents a worksheet for analysis of hazards within process systems. The paper concludes with an example of a liquefied natural gas (LNG) process system to illustrate the key concepts of this integrated approach.

- **Keywords:** Resilience; Process safety; Risk management; LNG; Organization; Human; System

Yunfeng Yang, Guohua Chen, Peizhu Chen. *The probability prediction method of domino effect triggered by lightning in chemical tank farm*. Pages 106-114.

A lightning strike is the main cause of fire accidents in chemical storage tanks, and the thermal radiation produced by a large storage tank fire may lead to a domino effect. A prediction method aiming to evaluate the probability of a domino effect at different levels triggered by lightning in the chemical tank farm is proposed. The developed method takes into account both the probability calculation model of fire triggered by lightning and the assessment method of the subsequent domino effect probability. Firstly, the accident scenarios and causes of fire triggered by lightning are analyzed by the event tree method, and a probability calculation model of fire accident triggered by lightning is developed. Secondly, the graph of chains of accidents is built considering synergistic effects and multi-level domino effects, and the Bayesian network is applied to calculate the probability of each accident chain. The most dangerous primary equipment is identified by comparison with the probabilities of the domino effect at different levels. By setting up the failure states of different tanks, the probabilities of events are updated under a given situation, and the most susceptible target equipment with respect to the domino effect are identified. Finally, the method is illustrated with two case studies in a

chemical industry park. The results will be helpful for the prevention of domino effects based on the theory of chain-cutting disaster mitigation.

- **Keywords:** Domino effect; Probability prediction method; Bayesian network; Lightning; Chemical tank farm

Somik Chakravarty, Marc Fischer, Pablo García-Triñanes, Morgane Dalle, Laurent Meunier, Olivier Aguerre-Chariol, Olivier Le Bihan, Martin Morgeneyer. *Long-term dust generation from silicon carbide powders*. Pages 115-125.

Most dustiness studies do not measure dust release over long durations, nor do they characterize the effect of dust release on bulk powders. In this study, we tested the dustiness of two different samples of silicon carbide (SiC) powders (referred to as F220 and F320) over six hours using a vortex shaker. Additionally, we characterized the bulk sample for change in shape and size distribution due to the testing. Both powders release respirable fractions of dust particles but differ in their dust generation behavior. The numbers of released respirable particles for powder F220 are more than two times higher than those of powder F320. The dust generation mechanism might include the release of aerosols due to the attrition of particles owing to inter-particle and particle-wall impaction. This study emphasizes the need for long duration dustiness tests for hard materials like SiC and characterization for change in bulk material properties due to dust generation and release. Furthermore, the results can aid in selecting the bulk material for long-term applications based on dustiness.

- **Keywords:** Dustiness; Silicon carbide particles; Vortex shaker; Attrition; Dust generation mechanism

Dinesh Kumar, Gaurav Kumar, Ram Das, Veena Agrawal. *Strong larvicidal potential of silver nanoparticles (AgNPs) synthesized using Holarrhena antidysenterica (L.) Wall. bark extract against malarial vector, Anopheles stephensi Liston*. Pages 137-148.

The present study highlights the strong larvicidal potential of silver nanoparticles (AgNPs) synthesized using bark extract of Holarrhena antidysenterica against third instar larvae of Anopheles stephensi over the other bark extract prepared in chloroform, hexane, ethyl acetate, methanol, aqueous and acetone individually. AgNPs were prepared by mixing of 90ml of silver nitrate (AgNO3) with 10ml of aqueous bark extract of H. antidysenterica. Optimization of various physical parameters such as temperature, pH, time duration and AgNO3 concentrations was done and 1mM of AgNO3, 7.5pH, 50±2°C temp and time 120min proved optimum for best synthesis of AgNPs. Characterized of AgNPs was done by ultraviolet-visible spectroscopy (UV–vis), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), field emission scanning electron microscope (FE-SEM) and transmission electron microscope (TEM). XRD pattern of such AgNPs revealed characteristics Bragg's reflection peaks at (38.34) 111, (44.54) 200, (64.36) 220 and (76.9) 311 lattice planes indicating the crystalline nature of biologically synthesized AgNPs. FT-IR analysis of AgNPs exhibited the presence of functional groups of various compounds including phenols, alcohols, amine, amide which were responsible for the reduction and capping of AgNPs. The FE-SEM and TEM images showed that most of the AgNPs were spherical, hexagonal and triangular in shape varying from 40 to 60nm in size. Larvicidal activity of these AgNPs and bark extracts prepared in different solvents such as hexane, ethyl acetate, methanol, water and chloroform were tested separately against the A. stephensi larvae for 24h. Maximum larval mortality was seen with bark extract synthesized AgNPs having LC50 and LC90 value of 2.672ppm and 4.482ppm, respectively compared to chloroform, hexane, ethyl acetate, methanol, water and acetone bark extracts where the LC50 values were 3.0, 31.56, 41.92, 96.40, 121.53 and

1.91E3ppm, respectively. Incidentally, AgNPs proved non-toxic against the non-target organism, Mesocyclops thermocyclopoides. GC–MS analysis of bark extract identified 41 compounds having a range of activities which might have helped in the bio-reduction of AgNPs. These AgNPs have tremendous applications in pharmaceutical and biomedical industries such as cancer therapies, targeted drug delivery, as antiseptic agents and as an imaging agent.

- **Keywords:** Anopheles stephensi; Silver nanoparticles; Holarrhena antidysenterica; Biosynthesis; Larvicidal activity

Jasmin Shah, Muhammad Rasul Jan, Fatima Khitab. *Sonophotocatalytic degradation of textile dyes over Cu impregnated ZnO catalyst in aqueous solution*. Pages 149-158.

To increase the performance of ZnO from UV to visible light, ZnO particles were impregnated with copper (Cu) using wet impregnation method. The synthesized impregnated ZnO was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), Fourier transformed infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS). The degradation of dyes with sonophotocatalytic process was high as compared to photocatalytic and sonocatalytic. The effects of the copper impregnated ZnO (Cu-ZnO) catalyst on the degradation of two textile dyes were investigated using the parameters like pH, catalyst dose, radical enhancer, radical scavenger and initial dye concentration. The addition of radical enhancer (H2O2) increased the degradation efficiency from 35% to 95% at pH 10. At optimum conditions, maximum degradation of dyes were 100% in 20min using sonophotocatalytic degradation as compared to photocatalytic process the degradation efficiency was 95–98% in 60min. With the addition of carbonate, sulphate and chloride as radical scavengers, the degradation efficiency decreased from 100% to 92%, 94% and 92% with 0.025M concentration of each scavenger, respectively. The degradation efficiency decreased only 5% after repeated use of Cu-ZnO catalyst. Therefore, Cu-ZnO catalyst can be used as a promising sonophotocatalyst for degradation of textile dyes with excellent reusability potential.

- **Keywords:** Sonophotocatalysis; Impregnated ZnO; Textile dyes; Degradation; Regeneration

Xinxiao Lu, Hongqing Zhu, Deming Wang, Chao Hu, Hongru Zhao, Yujia Huo. *Flow characteristic investigation of inhibition foam used for fire extinguishment in the underground goaf*. Pages 159-168.

Goaf fires are prevalent in underground coal mines and have drawn increasing public attention. Inhibition foam is recognized as an efficient means of fire extinguishment in a huge volume of porous material. A verisimilar goaf platform setup and a foam preparation system were developed. Experimental results show that increasing the gas/liquid ratio improves the foam stack effect. The optimum gas/liquid ratio and the ratio of infusion pipe length and cooling zone length are suggested for a practical application. The goaf interior pressure test indicates that the air leakage is controlled effectively by the inhibition foam. A perforated pipe will be superior to the standard one for a practical application due to its better diffusivity and lower infusion pressure.

- **Keywords:** Underground goaf; Fire extinguishment; Inhibition foam; Foam diffusion; Goaf pressure

Fei Li, Jingdong Zhang, Chaoyang Liu, Minsi Xiao, Zixian Wu. *Distribution, bioavailability and probabilistic integrated ecological risk*

***assessment of heavy metals in sediments from Honghu Lake, China*. Pages 169-179.**

Heavy metals (Cr, Cu, Zn, Pb, Cd) concentrations and fractions in surface sediments from Honghu Lake were detected by an atomic absorption spectrophotometer and Simple Bioavailability Extraction Test (SBET) from 11 typical sites to explore their spatial distribution, bioavailability and sources. Results showed the mean Igeos and ecological risk degrees decreased in the order of Cd>Cu>Cr>Pb>Zn and Cd>Cu>Pb>Cr>Zn. The metals' bioavailability estimated by SBET decreased in the general order of Cu>Pb>Cd>Zn>Cr. Under integrated consideration of metal enrichment, ecological risk and bioavailability, it obviously made the decision-makers confused to identify final priority pollutants and priority areas. Thus, a probabilistic integrated ecological risk assessment method (PIERA) was formulated based on the potential ecological risk index (PER), SBET and triangular fuzzy numbers for synthetically assessing metal enrichment, ecotoxicity and bioavailability. With the help of PIERA, Cd was finally regarded as the risk priority metal due to the integrated potential eco-risk of Cd made the average contribution of 86.4% to the integrated RIs. Moreover, the areas around S5 and S2 were regarded as the risk priority areas. The case application of PIERA revealed that this improved method is of a better resolving ability which scientifically supplies the integrated information of enrichment, bioavailability and systematic uncertainty for decision-makers compared with the other prevalent indexes (SQGs, Igeo, PER). The consequence of the Pearson correlation analysis, distribution analysis and field investigation indicated that Cd mainly originated from both non-point agricultural and industrial pollution sources.

- **Keywords:** Sediments; Heavy metals; Honghu Lake; Spatial risk assessment; Bioavailability; Triangular fuzzy numbers

Lin Li, Botao Qin, Dong Ma, Hui Zhuo, Hongjun Liang, Ang Gao. *Unique spatial methane distribution caused by spontaneous coal combustion in coal mine goafs: An experimental study*. Pages 199-207.

A new type of incident in the form of a methane explosion caused by spontaneous combustion of coal is receiving more and more attention due to the high ground temperature and high methane content in coal mines. To investigate the formation process of this type of incidents and advance the research on methane explosion risk caused by spontaneous coal combustion, a self-designed experimental platform was used to determine the influence of spontaneous coal combustion on methane migration in the goaf. Additionally, the effect of different ventilation velocities at the mining face on methane migration in the goaf was studied. The results reveal that air leakage plays a key role in methane migration in the goaf. The bigger the ventilation velocity, the larger the area affected by air leakage. In addition, the superposition of the air leakage and the horizontal and vertical movement of hot gases creates the entrainment effect in the spontaneous combustion area. Eventually, the methane concentration at the location of spontaneous combustion is the lowest and it gradually increases outside the spontaneous combustion area because of the superposition of air leakage, 'fire pressure' and the entrainment effect.

- **Keywords:** Spontaneous coal combustion; Methane explosion; Fire pressure; Air leakage; Entrainment effect

Zhenyi Liu, Yao Zhao, Tao Ren, Xinming Qian, Yi Zhou, Ruiyan Sun, Tao Li, Deping Zhang. *Experimental study of the flow characteristics and impact of dense-phase CO2 jet releases*. Pages 208-218.

High-pressure dense-phase CO2 transportation is the main approach for transportation of CO2 in China. During the transportation process, CO2 is in a high-pressure dense phase. If CO2 leakage occurs in such a case owing to line equipment damage, the low-temperature high-speed jet flow will be hazardous for human lives and property. To study CO2 leakage, an experiment was conducted to examine the impact of a dense-liquid CO2 jet during accidental releases. The impact value was measured for different nozzle sizes, inner pressures, and distances. Therefore, studying the mechanism and effectively evaluating the consequences and impact of the accidental leakage of high-pressure dense-phase CO2 are important for ensuring the security of its transportation.

- **Keywords:** Impact; Jet; Dense-phase; Carbon capture and storage; Flow characteristics

Lu-Qing Wang, Hong-Hao Ma, Zhao-Wu Shen, Dai-Guo Chen. *Experimental study of DDT in hydrogen-methane-air mixtures in a tube filled with square orifice plates*. Pages 228-234.

Deflagration to detonation (DDT) experiments with stoichiometric hydrogen-methane-air mixtures at ambient pressure (1atm) and temperature (293K) were carried out in a 112×112mm by 6m long tube with various obstacle configurations. The hydrogen fraction in fuel mixtures ranged from 0 to 1. Two types square orifice plates with opening sides of 86.8mm and 70.8mm (blockage ratios of 0.4 and 0.6), spaced at 1, 2, 3 and 4 times the tube height were employed. Flame signals were detected by photodiodes spaced evenly, from which the average velocity could determined. The detonation cell size was obtained using soot foil technique. CJ detonations can still propagate in less sensitive mixtures with larger detonation cell sizes. At the DDT limits, the ratio of the height of the orifice plate (d) and the detonation cell size (λ) increases with the increase of the blockage ratio and the decrease of obstacle spacing. This indicate that in a square tube with square orifice plates, the detonation initiation process as well as the detonation propagation mechanism govern the DDT limits.

- **Keywords:** Hydrogen-methane; Quasi-detonation; DDT limits; Explosions; Choked flame; Square orifice plates

Xin Zhang, Laibin Zhang, Jinqiu Hu. *Real-time diagnosis and alarm of down-hole incidents in the shale-gas well fracturing proces*. Pages 243-253.

Detecting down-hole incidents in the shale-gas well fracturing process plays an important role in ensuring that the fracturing operations are carried out smoothly. This paper proposes a method to monitor down-hole incidents by extracting the qualitative trend of process variables (QTPV) using qualitative trend analysis. This is based on the consideration that QTPV is similar at different magnitudes of down-hole incidents and that deviations from the normal pattern may indicate a possible incident. Based on this, this paper presents a real-time diagnosis and alarm method of down-hole incidents using a multi-class support vector machine (MCSVM) model for qualitative trend classification in real-time. Compared with the traditional modelling process in which process data is directly used as the input item to develop the MCSVM classifier, the proposed method can achieve higher global accuracy, as well as lower false and missing alarm rates, even with limited incident cases. Moreover, successful real-time diagnosis and alarm of down-hole incidents (cracks forming in the strata, channelling near the wellbore area, and sand plugs) are demonstrated. The results suggest that the presented method is a reasonable starting point for monitoring down-hole incidents during the shale-gas well fracturing process. This approach can be integrated into a real-time monitoring and alarm device for field application during fracturing operations.

- **Keywords:** Shale gas; Down-hole incident; Real-time diagnosis; Alarm; Qualitative trend

Tao Bu, Fu Chen, Xuemei He, Yang Yang, Wanlu Wang. *Researching the complexing conditions of residual boron in produced water from oil & gas fields*. Pages 254-261.

Large volumes of fracturing flowback fluids are generated as produced water (PW) during oil & gas extraction. There is a method that uses such produced water as a suitable source of fracturing water, recycling it into subsequent fracturing gels. Not only does it reduce processing costs and environmental pollution, but it also effectively alleviates the problem of oilfield water shortage. However, the existence of residual boron in PW is a crucial obstacle to reutilization because it prematurely crosslinks hydroxypropyl guar (HPG) that affects pumping and fracking. So it is necessary to eliminate the adverse effect of residual boron in terms of recycling PW. Fortunately, boric acid easily reacts with polyols by bonding with other active cis-hydroxyl groups to form complexes, preventing residual boron from prematurely crosslinking with HPG. This study demonstrated the feasibility of shielding residual boron crosslinker in PW by a series of simulated crosslink systems. Results indicate that mannitol has a high complexation capacity for boron since it forms stable 5-member ring complexes by bonding with borate ion. When the mole ratio of ligand to boric acid exceeds 2.5 and the pH value is around 10.5, the shielding efficiency of mannitol to boron reaches 95%. The excessive amounts of ligands completely shield the boron and prevent its continuous crosslinking with HPG. The fracturing gels prepared by PW no longer show the premature crosslinking phenomenon after the shielding agent is added, and its rheological properties loading the new crosslinker are similar to the system which is prepared with deionized water. These results indicate that mannitol can effectively shield the residual boron crosslinker, removing the adverse effects of premature crosslinking with HPG base fluid. This has formed stable complexes, which still exist in the HPG base fluid system and do not affect the rheological properties of the subsequent fracturing gels. Compared with conventional boron treatment technologies, this treatment system also directly prepares the subsequent fracturing gels without the additional steps of filtering boron-complexes. Therefore, there are many significant advantages in these operational steps over traditional boron removal methods from the perspective of efficiency and cost-effectiveness.

- **Keywords:** Fracturing flowback fluids; Recycling; Residual boron; Shielding agent; Complexation; Complexes

Imen Baklouti, Majdi Mansouri, Ahmed Ben Hamida, Hazem Nounou, Mohamed Nounou. *Monitoring of wastewater treatment plants using improved univariate statistical technique*. Pages 287-300.

Proper operation of the wastewater treatment plants (WWTPs) is crucial in order to maintain the sought effectiveness and desirable water quality. Therefore, the objective of this paper is to develop univariate statistical technique that aims at enhancing the monitoring of wastewater treatment plants using an improved particle filtering (IPF)-based multiscale optimized exponentially weighted moving average chart (MS-OEWMA). The advantages of the developed technique are fivefold: (i) estimate a nonlinear state variables of WWTPs using IPF technique. The IPF method yields an optimum choice of the sampling distribution, which also accounts for the observed data; (ii) use the dynamical multiscale representation to extract accurate deterministic features and decorrelate autocorrelated measurements. (iii) Develop an optimized EWMA (OEWMA) based on the best selection of smoothing parameter (λ) and control width L; (iv) combine the advantages of state estimation technique with MS-OEWMA chart to improve the fault detection in WWTP systems; and (v) investigate the effect of fault types (offset or bias, variance and drift) and fault sizes on the fault detection performances. The developed

technique is validated using simulated COST wastewater treatment BSM1 model. The BSM1, provided by the IWA Task Group on Benchmarking of Control Strategies, is a simulation platform that allows for creating sensor faults disturbances in a wastewater treatment plant. The detection results are evaluated using three fault detection criteria: missed detection rate (MDR), false alarm rate (FAR) and average run length (ARL1).

- **Keywords:** Improved particle filter (IPF); Exponentially weighted moving average (EWMA); Fault detection (FD); Wavelet representation; Wastewater treatment plant (WWTP)

Jiwan Singh, Byeong-Kyu Lee. *Effects of Nano-TiO2 particles on bioaccumulation of 133Cs from the contaminated soil by Soybean (Glycine max)*. Pages 301-311.

This study investigated the effects of nano-TiO2 particles on cesium uptake by soybean plant, which was conducted in a plant growth chamber with adding different concentrations of 133Cs to the soil. This study identified compositional and functional group changes of the elements contained in the soybean root and shoot due to the accumulation of 133Cs. With use of nano-TiO2, the accumulation of 133Cs identified in the shoot (731.7μg/g dw) was higher than that in the root (597.8μg/g dw). The Cs 3d peaks identified in the XPS spectrum analysis of the shoot and root biomass could be an evident for 133Cs accumulation. The appearance of the new FTIR peaks on the root and shoot biomass can be explained by new bond formation of 133Cs or nano-TiO2 with biomass matrix. Therefore, the application of nano-TiO2 in Cs contaminated soil can significantly enhance 133Cs uptake and its accumulation in plants.

- **Keywords:** 133Cs; Nano-TiO2; Accumulation; Soybean; XPS; FTIR

Sunday A. Adedigba, Faisal Khan, Ming Yang. *An integrated approach for dynamic economic risk assessment of process systems*. Pages 312-323.

This paper proposes a dynamic economic risk analysis methodology for process systems. The Bayesian Tree Augmented Naïve Bayes (TAN) algorithm is applied to model the precise and concise probabilistic dependencies that exist among key operational process variables to detect faults and predict the time dependent probability of system deviation. The modified inverted normal loss function is used to define system economic losses as a function of process deviation. The time dependent probability of system deviation owing to an abnormal event is constantly updated based on the present state of the relevant process variables. The integration of real time probability of system deviation with potential losses provides the risk profile of the system at any instant. This risk profile can be used as the basis for operational decision making and also to activate the emergency safety system. The proposed methodology is tested and verified using the Richmond refinery accident.

- **Keywords:** Dynamic failure prediction; Loss functions; Economic consequences; Process safety; Structure learning of Bayesian network from data and risk analysis

Christophe Bressot, Neeraj Shandilya, Thangavalu Jayabalan, Guillaume Fayet, Matthias Voetz, Laurent Meunier, Olivier Le Bihan, Olivier Aguerre-Chariol, Martin Morgeneyer. *Exposure assessment of Nanomaterials at production sites by a Short Time Sampling (STS) approach: Strategy and first results of measurement campaigns*. Pages 324-332.

Characterization of the exposition to nanoparticles and nano-objects at workplaces is a huge technical challenge. Workplace exposure during short durations is particularly

difficult to detect due to the low performances of the samplers. This article proposes a solution allowing for characterizing emissions at workplaces and presents the results obtained from a nanomaterials exposure measurement campaign performed on six different process lines (PLs) distributed all over Europe. By using our Short Time Sampling (STS) approach, the emitted nanomaterials are characterized in terms of their number concentration, size, shape and chemical composition. The background noise without any production activity is first measured for each PL and then it is distinguished from the emitted nanomaterials during production. The PLs yield different nanomaterial emission levels: the PL using the extrusion of polymer composites shows high emission whereas the PL dealing with the electrospinning of polyamide nanofibers shows the least i.e. no significant change in the background noise during the process and no detectable nanofiber emission either. The nanomaterials get emitted in the form of nanoparticles or submicronic fibers, or their agglomerates and aggregates i.e. Nano Objects, Agglomerates and Aggregates (NOAA). By the developed technique, 9 out of 37 of the studied steps have been shown to exhibit exposures to nanoparticles and nano-objects. For nanosafety measures, the energetic processes like spraying, extrusion, transport and cleaning activities of the nanomaterials in the powder form require most attention.

- **Keywords:** Nanoparticle; NOAA; Exposure; Measurement campaign; Short Time Sampling; Nanosafety; Risk assessment and management

Mohammad Hossein Keshavarz, Hamid Reza Pouretedal, Ehsan Saberi. *A novel method for predicting melting point of ionic liquids*. Pages 333-339.

For industrial applications, it is important to know phase transition properties such as melting points of ionic liquids (ILs). A novel correlation is introduced to predict melting points of important classes of ILs including imidazolium-, pyridinium-, pyrrolidinium-, ammonium-, phosphonium-, and piperidinium-based ILs and different type of anions with specific cation/anion moieties. It is based only on the number of some of atoms in cationic and anionic structures as well as two correcting functions for the presence of some specific cation/anion moieties. The numbers of carbon, hydrogen and nitrogen atoms are used for cation. Meanwhile, the numbers of hydrogen, nitrogen, bromine, chlorine and aluminum atoms are applied for anion. The measured data of 195 different types of ILs were used to derive the new correlations. The calculated coefficient of determination (R2), root mean square error (RMS), mean absolute error (MAE), mean absolute percent errors (MAPEs) and maximum of errors of the new model are 0.857, 26.1K, 20.1K, 6.5 and 91.2K, respectively. Meanwhile, the calculated RMS, MAE, MAPE and maximum of errors for one of the best available group contribution (GC) methods where it can be applied only for 159 ILs are 53.6K, 35.9K, 11.6 and 253.6K, respectively. For further 48 ILs with complex structure of cations and different anions, the values of RMS, MAE, MAPE and maximum of errors for the new model is also much lower than GC method. These results confirm that the reliability of the new model is good as well as it can be applied for a wide range of imidazolium-, pyridinium-, pyrrolidinium-, ammonium-, phosphonium-, and piperidinium-based ILs with different type of anions.

- **Keywords:** Ionic liquid; Melting point; Correlation; Structural parameter

Yu-duan Xie, Wan-li Xiong, Jun-xia Yu, Jia-Qi Tang, Ru-an Chi. *Recovery of copper from metallurgical sludge by combined method of acid leaching and biosorption*. Pages 340-346.

A novel combined acid leaching-biosorption process has been designed and applied to recover Cu from metallurgical sludge. Cu was firstly leached out and then selectively adsorbed from lixivium by using modified sugarcane bagasse (SCB) fixed-bed column. Leaching results by HNO3 showed that 96.9% Cu along with different leaching ratios of Mg, Ca, Zn, Fe, Cd, Pb, K and Cr were dissolved into the lixivium from the sludge. Three

types of breakthrough curve including inversed-L (for Mg, Ca, Fe, K and Cr), overshoot (for Zn, Cd and Pb) and S type (for Cu) were observed when the pretreated lixivium passing through the column, and adsorption kinetic results showed that the amount of Cu, Zn, Cd, Pb, Mg, Ca, Fe, K and Cr adsorbed was 16.6, 1.03, 0.04, 0.01, 0.03, 0.01, 0.77, 0.018 and 0.001mgg−1, respectively. Adsorption mechanism illustrated that Cu was selectively adsorbed from the lixivium due to its strong coordination ability with amine groups on the sorbent surface and the corresponding substitution reaction (between Cu and the co- ions). Cu could be recycled and the modified sorbent could be used repeatedly after column regeneration. These combined method had great potential in application of Cu recovery from sludge.

- **Keywords:** Copper; Metallurgical sludge; Sugarcane bagasse; Biosorption; Acid leaching

Jianfeng Zhou, Genserik Reniers. *A matrix-based modeling and analysis approach for fire-induced domino effects*. Pages 347-353.

Knock-on effects or so-called domino effects in the process industries may cause much greater losses than merely a primary event. Probability analysis of accidents resulting from domino effects is important for risk assessment. However, for the accident occurrence of a unit there may be mutual influences between the units in the area influenced by the accidents due to a domino effect, and this makes the calculation of probabilities of the accidents rather difficult. A matrix-based approach is proposed to model the influences between units influenced by a fire-induced domino effects, and the analysis approach for accident propagation as well as a simulation-based algorithm for probability calculation of accidents is provided. The synergistic effect of thermal radiation is taken into account during the accident propagation. The proposed approach is flexible to model and analyze domino effects in various conditions of primary fires by only changing the value of the initial matrix indicating the fire states. Two examples illustrate analyzing the fire propagation among tanks storing flammable liquids. The results show that this approach is simple but effective for offering an insight in the accident propagation process and for knowing the probabilities of equipment getting on fire.

- **Keywords:** Domino effect; Probability analysis; Matrix modeling; Process industry

Mohsen Naderpour, Nima Khakzad. *Texas LPG fire: Domino effects triggered by natural hazards*. Pages 354-364.

On February 2007, a massive fire in a propane de-asphalting unit in an oil refinery in Texas, USA happened due to liquid propane release from a cracked pipe in a control station injuring four people, damaging extensive equipment, causing significant business interruption, and resulting in more than $50 million losses. The accident was triggered by a natural hazard: freezing of piping at a control station caused an inlet pipe elbow to crack, which in turn, led to the release of high-pressure liquid propane which was rapidly ignited. In addition, there were two near-miss events due to potential domino effects. In fact, the accident could reasonably have resulted in much more severe consequences due to the exposure of large butane storage spheres and chlorine containers, increasing the possibility of a catastrophic domino effect. This paper develops a Natech (natural hazard triggering technological disasters) risk assessment methodology that relies upon Bayesian network capabilities and takes into account the potential Natech domino effects. The methodology is implemented in the intended refinery and mathematically graphically represents the dynamic cause–effect relations between units involved in the scenario, and handles uncertainties among the interactions. In addition, the methodology can provide a risk value for the entire scenario that can be used further for risk-based decision making.

- **Keywords:** Natech accident; Risk assessment; Domino effect; Bayesian network

Aydin Hassani, Alireza Khataee, Mehrangiz Fathinia, Semra Karaca. *Photocatalytic ozonation of ciprofloxacin from aqueous solution using TiO2/MMT nanocomposite: Nonlinear modeling and optimization of the process via artificial neural network integrated genetic algorithm*. Pages 365-376.

The degradation of ciprofloxacin (CIP) via photocatalytic ozonation process was investigated. TiO2 nanoparticles as an impressive photocatalyst were immobilized on the surface of montmorillonite (MMT). The main aim of the present work was to model and develop a relationship among the CIP degradation efficiency DE (%) and the key parameters affecting the complex photocatalytic ozonation process. The second object was to investigate the mutual effects of operating parameters on CIP DE (%) and express and optimum conditions that maximize CIP DE (%). To achieve these goals a nonlinear modeling and optimization of the process through artificial neural network (ANN) integrated genetic algorithm (GA) was successfully developed. The mutual effects of the input parameters including initial pH, ozone flow rate, initial CIP concentration, catalyst dosage and reaction time on CIP DE (%) were studied using the surface plots predicted with the nonlinear ANN model regarding the synergistic mechanism. GA was used as a nonlinear optimization method to determine the optimum conditions of input parameters. The good agreement between the experimental and GA predicted DE (%) under the optimum conditions confirmed that ANN integrated GA system is able to successfully model and optimize the photocatalytic ozonation performance.

- **Keywords:** Photocatalytic ozonation; Ciprofloxacin; TiO2/MMT nanocomposite; Nonlinear modeling; ANN-GA

Ahmad Jonidi Jafari, Roshanak Rezaei Kalantary, Ali Esrafili, Hossein Arfaeinia. *Synthesis of silica-functionalized graphene oxide/ZnO coated on fiberglass and its application in photocatalytic removal of gaseous benzene*. Pages 377-387.

Volatile organic compounds (VOCs) are a serious threat to public health, causing many serious diseases including cancer. Benzene is a VOC, causing different problems including aplastic anemia, acute leukemia, bone marrow abnormalities, and cardiovascular diseases in human who are exposed to it. Therefore, methods for degradation of benzene are required. In this study, for the first time silica-functionalized graphene oxide/ZnO (Silica-GO/ZnO) nano composite was synthesized and coated on fiberglass. It was then used for photocatalytic removal of benzene from the polluted air stream in a continuous reactor. The properties of the synthesized catalyst were examined by FTIR, XPS, XRD, SEM-EDX, N2 adsorption–desorption isotherms, and photoluminescence (PL) analyses, all of which confirming presence of silica and zinc oxide nanoparticles on graphene oxide, suggesting that GO-SiO2-ZnO photocatalyst was synthesized successfully. We investigated the effects of initial benzene concentration, flow rate, and humidity in degradation of benzene. The findings of this study indicated that the maximum removal efficiency of benzene was 87%. The range of optimal humidity for benzene removal was obtained as 35–45%. The results of this study showed that stabilization of ZnO on graphene oxide functionalized with silica has a significant effect in degradation of benzene from polluted air flow. The justification can be related to the fact that strong adsorption of benzene on GO results in further emission of pollutant to the ZnO catalyzer, thereby yielding a greater removal efficiency. With these results we can say the Silica-GO/ZnO is an efficient option for the elimination of benzene and biohazards emitted from industrial chimney streams.

- **Keywords:** Photocatalytic degradation; Nano-ZnO; SiO2; Graphene oxide (GO); Fiberglass; Benzene

Julio Idrovo-Novillo, Irene Gavilanes-Terán, Mª Angeles Bustamante, Concepción Paredes. *Composting as a method to recycle renewable plant resources back to the ornamental plant industry: Agronomic and economic assessment of composts*. Pages 388-395.

In this experiment, three piles were elaborated with rose waste (RW), sawdust (S), and different manures – broiler chicken manure (BCM), hen manure (HM), and quail manure (QM) – and were composted by windrow composting. Parameters associated with the degradation and humification of organic matter (OM) during composting and with the agronomic and economic value of the final composts were determined. All piles had temperatures >55°C for more than two weeks, ensuring compost sanitization. OM degradation was greater and faster in the pile with QM. This pile had the lowest water-soluble polyphenol content. Principal component analysis indicated that the use of BCM augmented the OM humification during composting; this material also influenced the mineralization of the OM. In general, the composts obtained presented an adequate level of stability and maturity and an absence of phytotoxicity, and there were notable concentrations of OM and nutrients, especially nitrogen. In addition, all the composts had an economic value when their nutrient contents were assessed. Phosphorus was the fertilization unit with the greatest contribution to the total value of the composts. However, the use of BCM produced a compost with properties that made it more suitable as an organic amendment for rose growing.

- **Keywords:** Flower waste; Composting; Compost maturity; Plant nutrient; Organic amendment; Economic value

A.F. Averill, J.M. Ingram, P.G. Holborn, P. Battersby, C.M. Benson. *Application of Bayesian methods and networks to ignition hazard event prediction in nuclear waste decommissioning operations*. Pages 396-404.

The major purpose of the study is to examine how Bayesian networks can be used to represent and understand potential ignition scenarios in nuclear waste decommissioning. This is illustrated using a network to represent a situation with stacked storage boxes containing pyrophoric material removed from waste storage silos. Corrosion of this material during storage produces hydrogen which is released through a filter medium into the gap between the boxes. The probabilistic relationships used to indicate dependence between network nodes are expressed by conditional probability tables or C++ coded equations that relate to UK nuclear industry corrosion and storage data. The study focuses on optimal prediction of the likelihood of a flammable hydrogen atmosphere arising in the gap between stacked boxes and the conditions necessary to exceed the lower flammable limit. It is concluded that the approach offers a useful means of easily determining the manner in which varying the controlling parameters affects the possibility of an ignition event. The effect of data variation can be examined at first hand using the supplementary Bayesian Network that accompanies the article.

- **Keywords:** Nuclear-waste; Magnox-corrosion; Hydrogen-ignition; Bayesian-Networks

Chao Wu, Wei Li, Peilun Xu, Sujing Li, Xiangqian Wang. *Hydrophobic mixed culture for 1,2-dichloroethane biodegradation: Batch-mode biodegradability and application performance in two-phase partitioning airlift bioreactors*. Pages 405-412.

Recent studies highlighted that hydrophobic microorganisms played key roles in VOC removal performance of two-phase partitioning bioreactors (TPPBs). The objective of this study was to evaluate the performance of a hydrophobic mixed culture for 1,2-

dichloroethane (1,2-DCA) biodegradation in both batch and TPPB tests. The hydrophobic mixed culture with cell surface hydrophobicity of 79% was acclimated from an activated sludge able to efficiently degrade 1,2-DCA as sole carbon and energy source. It was primarily composed of Xanthobacter genus (62%). Nearly complete degradation with coefficients of 0.80mgCO2mg1,2-DCA−1 and 0.66mgCl−mg1,2-DCA−1 was achieved for a wide range of 1,2-DCA concentrations (114.1–1141.5mgL−1) in the presence of silicone oil. The maximum specific growth rate was 0.247h−1 which was approximately two times the values of previous pure strains. The two-phase partitioning airlift bioreactors inoculated with the hydrophobic mixed culture was robust against step changes of gas flow rates and spike changes of inlet 1,2-DCA concentrations. All data proved the potential of the hydrophobic mixed culture for toxic-VOC removal in the TPPBs.

- **Keywords:** 1,2-Dichloroethane; Hydrophobic mixed culture; Batch-mode biodegradation; Kinetic analysis; Waste gas treatment; Two-phase partitioning airlift bioreactors

Akeem Adeyemi Oladipo. *MIL-53 (Fe)-based photo-sensitive composite for degradation of organochlorinated herbicide and enhanced reduction of Cr(VI)*. Pages 413-423.

Highly robust composite photocatalyst (WO3/MIL-53(Fe)) was synthesized and characterised. WO3/MIL-53(Fe) exhibits remarkable photocatalytic efficiency for reduction of Cr(VI) and oxidation of 2,4-dichlorophenoxyacetic acid (2,4-D) organochlorinated herbicide. After 240min sunlight irradiation, only ~30% reduction ratio of Cr(VI) was recorded in the presence of WO3. However, about 70% and 94% Cr(VI) reduction were achieved in the presence of MIL-53(Fe) and WO3/MIL-53(Fe), respectively. The removal efficiency proceeds more rapidly in the binary mixture of 2,4-D and Cr(VI) than in the single component system, indicating synergetic effect between the photooxidation and reduction reactions. O2− played a key role in the reduction of Cr (VI) and h+ is confirmed to be the dominant active species in the degradation of 2,4-D.

- **Keywords:** Metal–organic frameworks; MIL-53; WO3 nanoparticles; Cr(VI) reduction; Herbicide degradation

Mayur Shirish Jain, Mohit Daga, Ajay S. Kalamdhad. *Composting physics: A science behind bio-degradation of lignocellulose aquatic waste amended with inoculum and bulking agent*. Pages 424-432.

The composting is a proven technology to manage various organic wastes and reduces organic matter, heavy metals and harmful pathogens. The current research work provides the insight on the physics involved in composting of lignocellulose aquatic waste amended with inoculum and the bulking agent that plays a crucial role in handling, management, and utilization of waste product to an application of an end product in agriculture production. The physical parameters (temperature, bulk density, porosity, free air space, and particle density) during composting of E. Crassipes, inoculum and bulking agent (in the ratio 6:3:1) were evaluated. The study indicated an advanced thermophilic temperature (52.3°C) with 24% reduction in moisture content. As a result of volume reduction, the bulk density was found to be increasing whereas free airspace observed as 59% at the end of the composting process. The various physical parameters also exhibited the strong relationship to each other, which was derived using statistical analysis. The free air space correlated positively with bulk density and volatile solids.

- **Keywords:** Composting; Eichhornia crassipes; Moisture content; Oxygen availability; Free air space; Statistical correlation

Paolo Mocellin, Chiara Vianello, Ernesto Salzano, Giuseppe Maschio. *Pressurized CO2 releases in the framework of carbon sequestration and enhanced oil recovery safety analysis: Experiments and model*. Pages 433-449.

Hazard studies related to Carbon Sequestration (CCS) and Enhanced Oil Recovery (EOR) lack of appropriate descriptive models of pressurized CO2 releases. The complex inherent phenomena linked to a rapid depressurization in addition to the generalized lack of approachable and targeted experimental data, makes current QRA procedure inadequate. In light of this, the proposed work aims at achieving two correlated targets. Firstly, the results of an experimental campaign performed on CO2 pressurized releases are proposed. Secondly, a source model for multiphase CO2 pressurized releases is illustrated in terms of filling existing gaps. The reported experimental campaign focuses on the estimation of useful parameters to be used in the modeling procedure namely the experimental discharge coefficient and the thermodynamic nature of the expansion transformation. Bulk and discharge orifice pressure and temperature profiles are illustrated, focusing on how a multiphase CO2 release alters main discharge parameters. The proposed modeling approach allows for the collection of details on the expansion degree of reversibility and heat transfer effects are inferred showing that ideal isentropic and isenthalpic paths are never matched. Its application well matches collected data and gives good prediction of the total discharge time. In addition, direct unobservable dynamics inside the closed tank are assessed, notably the instantaneous dense CO2 mass fraction and peculiar evolutions during phase change mechanisms in the liquid-vapor and solid-vapor domains.

- **Keywords:** CCS safety; Vessel depressurization; Pipeline; CO2; Source model; QRA

N. M'hiri, R. Ghali, I. Ben Nasr, N. Boudhrioua. *Effect of different drying processes on functional properties of industrial lemon byproduct*. Pages 450-460.

The aim of this work was to investigate the effects of different drying processes on drying kinetics, physico-chemical properties and antioxidants of industrial lemon by-product. Lemon byproduct was submitted to infrared drying (50–75°C), convective drying (50–75°C), microwave drying (90–350W) and combined air-microwave drying (90W/50°C; 90W/75°C). Lemon byproduct is rich in water (3.18±0.12g water/g d.b), but also in phenols (5.52±0.08g GAE/100gd.b), with a radical scavenging activity of 8.381±0.400mg Trolox Equivalent/g of extract. The drying time of industrial lemon byproduct varies between 27min (350W) and 480min (infrared drying at 50°C). Combined-air microwave drying (590W/75°C) and convective air drying at 75°C allow better retention of phenols and flavonoids (more than 60%). Infrared drying of lemon byproduct at 75°C was in favour of maximal water and oil retention capacities and radical scavenging activity; whereas color preservation is achieved after microwave drying (90W) and convective drying (50°C).

- **Keywords:** Lemon byproduct; Drying kinetics; Oil and water retention; Antioxidants; Color

K.Y. Foo. *Effect of microwave regeneration on the textural network, surface chemistry and adsorptive property of the agricultural waste based activated carbons*. Pages 461-467.

This paper describes laboratory-scale experiments for examining the impact of microwave-irradiation on the regeneration of agricultural-waste based activated carbons loaded with methylene blue (MB). The efficacy of the regeneration study was analyzed by

determining the carbon yield and amount of MB adsorbed in successive adsorption–regeneration cycles. The virgin characteristics were examined by pore-structural-analysis, nitrogen adsorption-desorption curve, surface acidity/basicity and zeta-potential-measurement. Microwave heating preserved the porous structure of the regenerated activated carbons efficiently to restore the original activate sites and adsorption capacity, with the specific surface areas (SBET) of 605.88–711.74m2/g and monolayer adsorption capacities for MB of 199.74–231.68mg/g. Besides, the regeneration time was considerably shortened over conventional regeneration method, which represents a dramatic improvement in the adsorption chemistry.

- **Keywords:** Activated carbon; Adsorption; Methylene blue; Microwave; Regeneration

Yanlin Wu, Yahong Shi, Hongche Chen, Jianfu Zhao, Wenbo Dong. *Activation of persulfate by magnetite: Implications for the degradation of low concentration sulfamethoxazole*. Pages 468-476.

Sulfamethoxazole (SMX) was widely detected in the effluent of sewage treatment plants and water environment. In this study, SMX with low concentration was effectively degraded by magnetite-activated persulfate (PS) system. The process mainly involved the sulphate radical (SO4−) and hydroxyl radicals (HO), formed from PS activated by Fe(II) and Fe(III) in Fe3O4. The second-order reaction rate constants for the reaction between SMX and HO/SO4− were estimated. The SMX degradation rate decreased as the solution pH increased from pH 3.5–10.5 and the pH dependency of SMX degradation rate was closely related to the speciation of Fe2+. HO, SO4− and O2− were involved during PS activation. The effects of chloride were investigated. SMX degradation efficiency was significantly decreased due to the trapping of SO4− by Cl− at pH 4.0, while it had no effect by Cl− at pH 10.5 due to the formation of HO. The potential recyclability of Fe3O4 was measured and it could be reused at least 4 times. The findings may have promising implications in the application of Fe3O4 on a new technology for the treatment of micro-contaminated waters and soils, especially the application of natural magnetite.

- **Keywords:** Persulfate; Magnetite activation; Reaction rate constants; Chloride effect; Reuse

Soraya Hosseini, Soorathep kheawhom, Salman Masoudi Soltani, Mohamed Kheireddine Aroua, Houyar Moghaddas, Rozita Yusoff. *Improvement of product selectivity in bicarbonate reduction into formic acid on a tin-based catalyst by integrating nano-diamond particles*. Pages 494-505.

In this study, the efficiency of electrochemical reduction of bicarbonate into formic acid was improved by using a composite electrode made up of tin (Sn), nanodiamond (ND) and carbon nanotube (CNT). In the absence of ND, a compositional ratio of 10/90 (Sn/CNT) demonstrated the highest current density. However, by adding ND in a compositional ratio of 10/90/100 (Sn/CNT/ND) the highest efficiency towards formate/formic acid was achieved. It was observed that the presence of ND enhanced the selectivity of product for formic acid. The effects of bicarbonate concentration and scan rate have also been studied to understand the reduction mechanism. The peak potential shifted towards larger negative values of applied potential with an increase in the scan rate from 0.01 to 0.1V/s, confirming the irreversible nature of the reduction process. The linear relationship between the current and the square root of the scan rate (with a slope value of 0.519) suggested that the reaction process is fully diffusion-controlled. Formic acid was produced using both electrodes; however, the electrode containing nano-diamond successfully improved the process yield for formic acid. Electrochemical impedance study revealed a significant difference between Warburg coefficient for

oxidation and reduction processes with values of 29.63×1012 and 67.4Ω.S−0.5 for the applied potentials of 0.5V and −0.4V, respectively. This difference confirmed a low resistance at the electrode/electrolyte interface for the reduction potentials.

- **Keywords:** Bicarbonate (HCO3-); Composite electrode; Electrochemical reduction; Formic acid; Nano-diamond; Tin

M. Elazzouzi, A. El Kasmi, K. Haboubi, M.S. Elyoubi. *A novel electrocoagulation process using insulated edges of Al electrodes for enhancement of urban wastewater treatment: Techno-economic study*. Pages 506-515.

A comparison between conventional process and novel process of insulated edges electrodes in a batch electrocoagulation (EC) reactor for the treatment of urban wastewater was undertaken to investigate the effect of current density, operating time and initial temperature on the treatment efficiency. The optimal experimental conditions are found to be: current density of 20mAcm−2, operating time of 6min and initial temperature of 45°C for phosphorous (P) and 55°C for chemical oxygen demand (COD). The high removal efficiencies of COD and P using conventional electrodes system were found to be 89% and 99%, respectively. By comparison, the removal efficiencies using insulated edges of electrodes were achieved 91% for COD and 99.5% for P. The adsorption capacities of COD and P for conventional and novel processes were found to be 5930mg CODkg−1 and 80mgPkg−1, and 5860mg CODkg−1 and 77mgPkg−1, respectively. The sludge generated at optimum operating conditions using conventional and novel processes were calculated as 1.5kgm−3 and 1.8kgm−3, respectively. Also, insulated electrode process exhibited the ability to reduce the cost to 0.62$kg−1 for COD and to 0.58$kg−1 for P. The characterization study of produced sludge confirms that metal hydroxides and oxyhydroxides constitute the main components that contributed strongly to remove COD and P from urban wastewater.

- **Keywords:** Urban wastewater; Electrocoagulation (EC); Operating cost; Sludge characterization; Insulated edges electrodes

F. Lucernoni, L. Capelli, V. Busini, R. Del Rosso, A.A. Prata, R. Stuetz, S. Sironi. *Investigation of mass transfer phenomena affecting emission rate of gaseous compounds from porous solids*. Pages 516-526.

The main objective of this study is to investigate the mass transfer phenomena affecting the emission of acetone from a porous solid. In order to simulate this type of emission in a laboratory-scale and in a repeatable way it was decided to set up a system consisting of a dry solid layer with an underlying wet layer. This type of investigation aims to give a scientific basis for the understanding of the factors affecting emission rates when sampling solid area sources with a wind tunnel system. This in turn is important in order to make results obtained with different devices somehow comparable. The study was carried out by following a modellistic and an experimental approach, and then comparing the results. The comparison of experimental and modelled results shows a good agreement, proving that the developed model is able to describe the phenomenon, thereby taking into account the phenomenon intra-solid gas diffusion, as well as capillary rise of the liquid. As a final result, the proposed model is capable to describe properly how the emission rate from a porous solid is affected by the sweeping airflow velocity, which was the final purpose of this study. Although the developed model is valid for the simplified experimental set-up studied (consisting of a dry solid layer with an underlying wet layer and involving the use of pure acetone), the understanding of the phenomena affecting mass transfer in this simplified situation can be transferred to the investigation of diffusion of other compound through more complex solids.

- **Keywords:** Gaseous emissions; Liquid area sources; Solid area sources; Odorants; Hood sampling; Wind tunnel; Mass transfer; Source term

J.S. Binoj, R. Edwin Raj, S. Indran. *Characterization of industrial discarded fruit wastes (Tamarindus Indica L.) as potential alternate for man-made vitreous fiber in polymer composites*. Pages 527-534.

Environmental degradation and its effects on human health due to unprecedented use of synthetic fibers, have been heavily felt by the fabricating workers and by the common people in general. The search to develop high-performance materials using environmental friendly natural fibers, is to be encouraged and needs comprehensive characterization. In this paper, discarded and polluting agro waste from food processing industry, known as Tamarind Fruit Fiber (TFF) is tested for its potentiality as a reinforcement in polymer composite. The extracted fibers are subjected to anatomical, physical, mechanical, morphological, thermal and chemical examination. The low density (1.27g/cm3) provides high strength (1137–1360MPa), better thermal stability (238°C) and superior bonding characteristics revealed by standard investigations promotes TFF as a promising natural fiber reinforcement for many composite applications. Low cost and competent performance can be achieved with this natural fiber when reinforced in polymer matrix.

- **Keywords:** Discarded waste; Polymer composites; Physical properties; Chemical properties; Mechanical properties; Thermal properties

Hafida Lebik-Elhadi, Zacharias Frontistis, Hamid Ait-Amar, Said Amrani, Dionissios Mantzavinos. *Electrochemical oxidation of pesticide thiamethoxam on boron doped diamond anode: Role of operating parameters and matrix effect*. Pages 535-541.

The electrochemical oxidation of the neonicotinoid pesticide thiamethoxam (TMX) on a boron-doped diamond (BDD) anode was investigated. The effect of several operating parameters such as supporting electrolyte (0.025-0.1M Na2SO4, 0.1M NaCl), current density (4–40mAcm−2), TMX concentration (1–10mgL−1 of active ingredient in a commercial formulation) and initial solution pH (3–11) on degradation was evaluated. The apparent rate constant of a pseudo-first order kinetic model was found to increase with increasing (i) current density (from 0.036 to 1min−1 at 4 and 40mAcm−2, 2mgL−1 TMX and 0.1M Na2SO4) and (ii) Na2SO4 concentration (from 0.037 to 0.25min−1 at 0.025 and 0.1M Na2SO4, 2mgL−1 TMX and 16mAcm−2 current density) and decreasing (iii) TMX concentration (from 0.05 to 0.73min−1 at 10 and 1mgL−1 TMX, 0.1M Na2SO4 and 16mAcm−2 current density) and (iv) initial solution pH (from 0.017 to 2.13 at pH 11 and 3, 0.1M Na2SO4, 2mgL−1 TMX and 16mAcm−2 current density). Experiments in actual matrices, such as secondary treated wastewater and bottled water, resulted in lower kinetics (0.02 and 0.04min−1, respectively) than in pure water (0.22min−1), signifying competitive interactions between TMX and the matrix constituents. Of the latter, organic matter (1–15mgL−1 in the form of humic acid), bicarbonates (>100mgL−1) and chlorides (>100mgL−1) all had a detrimental effect on degradation. The rate constant of TMX degradation in pure water was reduced by 82%, 71% and 36% in the presence of 15mgL−1 humic acid or 500mgL−1 bicarbonates or 500mgL−1 chlorides, respectively. Fast TMX degradation (i.e. complete removal of 2mgL−1 TMX in 20min at 16mAcm−2, 0.1M Na2SO4, in pure water) is accompanied by slower mineralization (i.e. 91% total organic carbon removal at 120min), indicating the formation of more resistant transformation by-products.

- **Keywords:** Commercial product; Kinetics; Pesticide; Water composition; Neonicotinoids; Thiamethoxam; Anodic oxidation

R. Miandad, M.A. Barakat, M. Rehan, A.S. Aburiazaiza, J. Gardy, A.S. Nizami. *Effect of advanced catalysts on tire waste pyrolysis oil*. Pages 542-552.

Abstract: This study aims to examine the effect of various advanced catalysts on tire waste pyrolysis oil using a small pilot-scale pyrolysis reactor with a capacity of 20L. The catalytic pyrolysis with activated alumina catalyst produced maximum liquid oil (32wt.%) followed by activated calcium hydroxide (26wt.%), natural zeolite (22wt.%) and synthetic zeolite (20wt.%) catalysts, whereas liquid oil yield of 40% was obtained without catalyst. The gas chromatography-mass spectrometry results confirmed the pyrolysis liquid oil produced without catalyst consist of up to 93.3% of mixed aromatic compounds. The use of catalysts decreased the concentration of aromatic compounds in liquid oil down to 60.9% with activated calcium hydroxide, 71.0% with natural zeolite, 84.6% with activated alumina, except for synthetic zeolite producing 93.7% aromatic compounds. The Fourier-transform infrared spectroscopy data revealed that the mixture of aromatic and aliphatic hydrocarbon compounds were found in all liquid oil samples, which further confirmed the gas chromatography results. The characteristics of pyrolysis liquid oil had viscosity (1.9cSt), density (0.9g/cm3), pour point (−2°C) and flash point (27°C), similar to conventional diesel. The liquid oil had higher heating values, key feature of a fuel, in the range of 42–43.5MJ/kg that is same to conventional diesel (42.7MJ/kg). However, liquid oil requires post-treatments, including refining and blending with conventional diesel to be used as a transport fuel, source of energy and value-added chemicals.

- **Keywords:** Tire waste; Pyrolysis; Catalyst; Liquid oil; Transport fuel

Swapnila Roy, Shubhalakshmi Sengupta, Suvendu Manna, Papita Das. *Chemically reduced tea waste biochar and its application in treatment of fluoride containing wastewater: Batch and optimization using response surface methodology*. Pages 553-563.

Pyrolysis of domestic tea waste was carried out to yield bio-char which was further chemically treated using Hummer's method to form carbonaceous materials. Hummer's method is generally used to prepare graphene oxide (GO) from carbon source and it was observed from XRD, SEM and FTIR analysis that the structure of the synthesized biochar is similar to reduced GO. The adsorbent thus obtained was further applied for the treatment of fluoride containing simulated effluent. Effect of different experimental parameters on the fluoride removal efficiency using chemically reduced biochar and only tea waste biochar were investigated. Data obtained was further used for determination of process isotherms, kinetics and thermodynamics. The experimental results suggested that equilibrium adsorption data was strongly guided by the Langmuir isotherm and pseudo-second-order kinetics. Significant process parameters were optimized using Response surface methodology (RSM). Under optimized conditions, fluoride removal efficiency using chemically reduced biochar was found to be 98.31%.

- **Keywords:** Tea waste; Biochar; Graphene oxide; Ultrasonication; Fluoride removal; Process optimization; Response surface methodology

Shoujun Li, Xiaoping Ma, Chunyu Yang. *Prediction of spontaneous combustion in the coal stockpile based on an improved metabolic grey model*. Pages 564-577.

Spontaneous combustion of coal can lead to serious environmental pollution, safety hazards and huge economic losses. Hazard prevention and environmental protection requires effective monitoring network and efficient prediction methods. To acquire the real-time data of coal parameters we designed multi-layered Zig-bee based wireless

sensor network. The shape of the coal pile is formed by the industrial laser scanner followed by the formation of 3D temperature point cloud field via Kriging interpolation. Afterwards, an integrated evaluation indicator Heat Loss Capacity (HLC) is proposed, which synthesizes various factors inducing spontaneous combustion. The real-time and high accurate HLC prediction is realized by using metabolic method to update the raw sequence of the GM(1,1) grey prediction model in cycle with the latest acquired sensor data. Finally, a hybrid model ABC-MGM(1,1) combining the ABC optimization algorithm with the metabolic GM(1,1) model is proposed. Experiment shows that the ABC-MGM(1,1) model has better performance in parameter optimization as well as HLC prediction, especially for short-term prediction. The proposed method has been utilized to predict spontaneous combustion of the stockpiled coal in Xutang power plant of China. The timely parameter acquisition by 25 Zig-bee nodes and effective prediction by the proposed model shows great practicability in safety and hazard prevention.

- **Keywords:** Prediction of spontaneous combustion; Artificial bee colony algorithm; Metabolic GM(1, 1) model; Particle swarm optimization; Genetic algorithm; Environmental protection

Kamel Hendaoui, Fadhila Ayari, Iyadh Ben Rayana, Raja Ben Amar, Fadhila Darragi, Malika Trabelsi-Ayadi. *Real indigo dyeing effluent decontamination using continuous electrocoagulation cell: Study and optimization using Response Surface Methodology*. Pages 578-589.

In the present study, the response surface methodology (RSM) model was applied to study and perform the treatment of real indigo dyeing effluent by continuous electrocoagulation process using iron electrodes. The main effect of three parameters: initial pH, inlet flow rate and applied voltage along with their interaction on pollutants removal were evaluated. Results show that the increase of applied voltage and the decrease of inlet flow rate enhance the efficiencies of the pollutants removals. According to P values and analysis of variance ANOVA, there is a good adjustment between the second order regression models and experimental data for all responses. From surface plot analysis, it was well observed that the best pollutants removals were achieved at neutral pH range with the lowest flow rate and the highest voltage. When the conductivity removal was neglected, with the optimal parameters values: 7.58pH, 1L/min inlet flow rate and 101V applied voltage the color and COD removal were achieved as 93.77% and 92.07% respectively (fixed target equal to 95%). However, at optimum EC conditions: pH 7.2, inlet flow rate 1.1L/min and 66V applied voltage: 89.2%, 76.1% and 29.76% of color, COD and conductivity removal were achieved respectively with only 0.527 US$ per m3 of treated effluent as total cost. In the actual study, with the EC process the conductivity removal was improved by 60% compared with the actual biological used process.

- **Keywords:** Response surface methodology; Treatment; Electrocoagulation process; Effluent; Real indigo; SITEX company

Leila Omidi, Seyed Abolfazl Zakerian, Jebraeil Nasl Saraji, Esmaeil Hadavandi, Mir Saeed Yekaninejad. *Safety performance assessment among control room operators based on feature extraction and genetic fuzzy system in the process industry*. Pages 590-602.

Abstract: Human factors were identified as root causes and contributing factors of major accidents and can affect safety performance. The aim of this study was to model and work on human factors elements affecting safety performance of control room operators in the oil industry in Iran using a hybrid intelligent approach. Safety performance among control room operators regarding human factors issues was considered in the field and a hybrid intelligent model was employed to model the obtained data. The valid

questionnaire containing 283 items in 28 dimensions was used to evaluate safety performance. A hybrid intelligent model in three stages was used to estimate safety performance among control room operators. In the first stage, principal components analysis (PCA) was used to extract 28 main dimensions from related items in the questionnaire. In the second stage, correlation-based feature selection (CFS) was applied to identify the most important dimensions (features) affecting safety performance. In the third stage, genetic fuzzy system was employed for modeling safety performance by selected dimensions as input variables. The feature selection method showed that human-computer interface, manual materials handling, safety culture, safe work practices and permit–to–work systems, quantitative risk analysis, competence management, and incident investigation were the subsets with the highest merit values. The results of genetic fuzzy system revealed that, among features with the highest merit values, safe work practices and permit–to–work systems, human-computer interface, and staff competence had major effects on safety performance of control room operators.

- **Keywords:** Safety performance; Human factors; Process industry; Genetic fuzzy system; Hybrid intelligent model

Shang-Hao Liu, Wei-Cheng Lin, Han Xia, Hung-Yi Hou, Chi-Min Shu. *Combustion of 1-butylimidazolium nitrate via DSC, TG, VSP2, FTIR, and GC/MS: An approach for thermal hazard, property and prediction assessment*. Pages 603-614.

Abstract: Ionic liquids (ILs) possess negligible vapor pressure, a low toxicity, a low melting point, and a vast liquid temperature range, rendering them as favorable candidates for new alternative solvents. However, some recent studies showed that ILs are flammable during thermal upsets. To explore the overall spontaneous combustion under upset conditions, we propose a safer method to investigate the IL's thermal hazards. Gas chromatography/mass spectrometry, Fourier transform infrared spectrometry, and flash point analysis results indicated that 1-butylimidazolium nitrate ([BIM][NO3]) exhibits combustible characteristics and low thermal stability at high temperatures (over ca. 150.0°C) during thermal decomposition. Meanwhile, differential scanning calorimetry, thermogravimetry, and vent sizing package 2 (VSP2) tests were used to describe the thermal properties of [BIM][NO3]. The thermokinetic parameters were further acquired by using an isoconversional method. The results demonstrate that the suitable combination of anion and cation might yield energetic ILs.

- **Keywords:** Ionic liquids (ILs); Gas chromatography/mass spectrometry; Fourier transform infrared spectrometry; Combustible characteristics; Isoconversional method

Almerinda Di Benedetto, Roberto Sanchirico, Valeria Di Sarli. *Effect of pressure on the flash point of various fuels and their binary mixtures*. Pages 615-620.

The effect of pressure on the flash point (FP) of various fuels (methanol, ethanol, acetone, ethyl acetate, n-hexane, n-octane, benzene, toluene) and their binary mixtures (ethanol-acetone, ethanol-n-octane, methanol-hexane) has been quantified. It has been found that the FP significantly decreases with decreasing pressure. In particular, in going from 1atm to 0.4atm, the FP decreases of about 10°C for all the pure substances investigated. This means that, when dealing with industrial processes operated at pressure lower than 1atm, the FP present on the material safety data sheet is not conservative since it is measured at 1atm. A unique equation for evaluating the FP at different pressures starting from the value at atmospheric pressure has been proposed and validated. This equation applies to both pure substances and their binary mixtures, both ideal and non-ideal.

- **Keywords:** Flash point; Pressure; Correlation; Binary mixtures; Safety

Valeria Casson Moreno, Genserik Reniers, Ernesto Salzano, Valerio Cozzani. *Analysis of physical and cyber security-related events in the chemical and process industry*. Pages 621-631.

Security threats are becoming an increasing concern for chemical sites and related infrastructures where relevant quantities of hazardous materials are processed, stored or transported. In the present study, security related events that affected chemical and process sites, and related infrastructures, were investigated. The aim of the study is to frame a clear picture of the threats affecting the chemical and process industry, and to issue lessons learnt from past events. A database of 300 security-related accidents was developed and populated, starting from European and American sources. Threat categories that caused such events were identified and analyzed. The attack modes were investigated. Important differences were found with respect to geographical areas and industrial sectors affected. The use of explosives (both military and improvised explosive devices) is by far the more frequent attack mode, although armed attacks and arson are also frequent events and may result in an in-depth penetration of the attackers. In recent years, cyber-attacks are also posing important threats. Lessons learnt call for the implementation of a specific security management system in the chemical and process industry, aiming at the physical and cyber protection of industrial sites.

- **Keywords:** Security; Cyber; Attacks; Threat; Incidents; Accidents; Chemical and process industry

Jin Wang, Tingting Xiao, Ruyi Bao, Tao Li, Yanqiang Wang, Dengxin Li, Xuemei Li, Tao He. *Zwitterionic surface modification of forward osmosis membranes using N-aminoethyl piperazine propane sulfonate for grey water treatment*. Pages 632-639.

Zwitterionic amide monomer (N-aminoethyl piperazine propane sulfonate, AEPPS) was used to modify the active layer of the thin-film composite (TFC) Forward Osmosis Membranes (FOMs) by either adding into the water phase before the interfacial polymerization (route 1) or grafting to the initial active separation layer after the interfacial polymerization (route 2). Their separation performance and anti-fouling property were investigated. Different from the literature results, the synthesized AEPPS was a mixture of isomers which is too complicated to be purified. Results showed that both fourier transform infrared spectroscopy and X-ray photo-electron spectroscopy confirmed that the zwitterionic materials were successfully incorporated into the FOMs. However, in a long-term FO fouling test by using grey wastewater as the feed solution, surface grafted zwitterionic FO membrane prepared after the interfacial polymerization (route 2) showed superior stable FO performance than the membrane prepared by imbedding the AEPPS inside the active layer (route 1). Imbedded AEPPS chemical inside the active layer could not prevent the adsorption of foulant, thus no relief in the fouling was observed. The results demonstrated that the zwitterionic material surface grafting after the interfacial polymerization way is a more efficient approach to prepare fouling resistant FOMs for treating greywater.

- **Keywords:** Forward osmosis; Zwitterionic; Greywater; Thin-film composite; Interfacial polymerization

Ziwei Ye, Fan Yang, Yiqin Qiu, Nanwei Chen, Weixiong Lin, Shuiyu Sun.. Pages 654-662. *The debrominated and lightweight oil generated from two stage pyrolysis of WPCBs by using compound chemical additives*

The effect of employing compound additives were investigated for application to the catalytic pyrolysis of waste printed circuit boards (WPCBs), in order to recycle low brominated and lightweight oils. The study included the analysis of three-phase product yields; organic and inorganic bromine distributions; oil content; and the boiling point of experimental product fractions. Bromine distributions were analyzed using ion chromatography (IC) and oxygen bomb calorimeter, with oil products analyzed using gas chromatography-flame ionization (GC/FID) and gas chromatography-mass spectrometry(GC/MS). Results show that the pyrolysis liquid up to 27.04wt.% by using CaCO3+4A; the total bromine content(include organic and inorganic) of pyrolysis liquid was reduced to 4.68wt.% through Fe3O4+4A; Using Fe3O4+Al2O3 can increase the water content(68.76wt.%) of pyrolysis liquid; the application of Fe3O4+4A can cut down the organic bromine to 1.59wt.%; Fe3O4+5A can increase the 150–200°C fraction(gasoline) to 53.25%; the phenol fraction can be increased to 46.01% applied Fe3O4+5A; the bromophenol less than1.30% and bisbromophenol was not detected. Thererfore, using Fe3O4+5A to recycle the low brominated and lightweight pyrolysis oil have a huge significance,which can use as potential fuel.

- **Keywords:** WPCBs; Compound chemical additives; Two stage pyrolysis; Debomination; Lightweight oil

T. Li, F. Hampp, R.P. Lindstedt. *Experimental study of turbulent explosions in hydrogen enriched syngas related fuels*. Pages 663-676.

Abstract: The role of hydrogen enriched fuel streams has come to the fore due to the use of syngas and/or biogas related feedstocks in gas engine or gas turbine based power generation applications. The hydrogen addition can enhance the fuel reactivity significantly, leading to improved combustion stability and widened flammable limits, but also raises safety concerns related to accidental explosions. The current work presents a systematic study of turbulent deflagrations generated in an obstructed tube with explosion overpressures and flame speeds measured. The focus is on the use of lean and ultra-lean fuel blends using binary H2/CO, H2/CH4 and ternary H2/CH4/CO mixtures. The H2 levels were varied between 0% and 100% at stoichiometries of 0.80, 0.60 and 0.40. The results highlight significant differences in explosion behaviour between the two blending components, with CO mixtures providing substantially higher overpressures than the corresponding CH4 blends. The results suggest that methane has a mitigating effect up to comparatively high hydrogen blending fractions and that synergistic effects between fuel components need to be taken into account. A new scaling parameter (β) is proposed that successfully linearises the peak explosion overpressure between different fuel blends in response to the hydrogen concentration. A scaling based on acoustic theory shows good agreement with experimental data and a simple method for estimating the overpressure change caused by variations in the mixture reactivity in a fixed geometry is also evaluated.

- **Keywords:** Hydrogen enrichment; Syngas; Explosions; Fuel lean blends; Scaling

V.S. Smitha, J. Samuel Vara Kumar, M. Surianarayanan, H. Seshadri, N.V. Lakshman. *Reactive chemical pathway of tributyl phosphate with nitric acid*. Pages 677-684.

Tributyl phosphate and its degradation products saturated with nitric acid and exposed to elevated temperatures lead to an accidental condition known as "reactive red oil formation". The present study aims at elucidating the chemical pathway of this reaction in an Accelerating Rate Calorimeter (ARC). The thermal characteristics obtained from ARC coupled with end product analysis using spectroscopic techniques proved that red-oil forming mechanisms varied as per the concentration of nitric acid. The chemical pathway for red oil formation was found to occur through the oxidation of butanol at lower temperatures and with dilute nitric acid, the predominant path was via butyl nitrite

intermediate at higher temperatures. Independent ARC experiments with butanol and butyl nitrite with nitric acid validated the mechanism. This study also revealed that most of the diluents employed for TBP undergo exothermic reaction with nitric acid, even in the absence of TBP.

- **Keywords:** Tri butyl phosphate; Nitric acid; Diluents; Accelerating rate calorimeter; Thermal hazards; Reaction pathway

Marcela Marcondes de Santana, Everton Fernando Zanoelo, Cristina Benincá, Flavio Bentes Freire. *Electrochemical treatment of wastewater from a bakery industry: Experimental and modeling study*. Pages 685-692.

The typical treatment of wastewater from the bakery industry in skimming tanks and bioreactors has some limitations, such as low removal of grease, and partial degradation of organic matter. The primary aim of this investigation was to evaluate the use of electrocoagulation as an alternative/complementary method to treat efficiently such an effluent, with focus on the determination of the best operating conditions, and on the kinetics of electrocoagulation at the optimal defined set of process variables. To search for the optimal, a 23 factorial design of electrocoagulation experiments with iron and aluminum electrodes was applied in the pH range from 4.6 to 7.0, at 6 and 12V for 1200s and 2400s. A reliable statistical model revealed that the results of removal of chemical oxygen demand (6–8%) and turbidity (32–98%) by using aluminum electrodes, which were in average about twice as high as those with iron electrodes, were influenced by almost all the considered factors ($p \leq 0.05$). At the best determined values of pH (7.0) and voltage (12V), kinetic experiments of electrocoagulation with aluminum electrodes were performed by monitoring periodically the pH, turbidity, apparent color, concentration of oil/grease, chemical oxygen demand, concentration of chloride anion and electric conductivity of the wastewater for 2400s. Almost all the examined pollutant parameters, and in particular the content of oil/grease (traditionally poorly removed in fat traps) were reduced to negligible values in a short treatment time. A reliable semi-empirical kinetic model described properly the high rates of disappearance of turbidity and apparent color.

- **Keywords:** Bakery; Wastewater; Electrocoagulation; Statistical model; Kinetic model

Munmun Banerjee, Ranjan Kumar Basu, Sudip Kumar Das. *Cr(VI) adsorption by a green adsorbent walnut shell: Adsorption studies, regeneration studies, scale-up design and economic feasibility*. Pages 693-702.

Natural water resources are polluted due to human activities like discharge from municipal and industrial wastewater. In general industrial wastewater contains toxic chemicals like heavy metals, dyes, acids etc. To save the water bodies it is necessary for industries to treat their wastewater before disposal. Agricultural wastes like green adsorbents may be considered as an alternative to minimize the problems regarding heavy metal pollution particularly for small and medium sized industries. In this study walnut shell, an agricultural waste is used for Cr(VI) removal as green adsorbent. Brunauer-Emmett-Teller (BET), Scanning electron microscopy (SEM), Point of zero charge (pHpzc) and Fourier transform infrared spectroscopy (FTIR) were used to characterise the walnut shell. Column studies were performed for different operating conditions and low influent flow rate, low influent Cr(VI) concentration and higher bed depth give better adsorption. Langmuir isotherm model fitted well for Cr(VI) adsorption equilibrium (KL=0.6754L/mg, R2=0.9996). Different kinetic models are applied on experimental data to evaluate model parameters and their applicability. Yan et al. model

fitted well for the specified operating range (KY=5903.63mL/(mgmin), R2=0.9785) and applied for scale-up designing. Regeneration studies are conducted by using different concentration of NaOH to investigate the reusability characteristics of walnut shell. Scale-up design for Cr(VI) removal using walnut shell as an adsorbent and its economic feasibility are done to find out its applicability in real life. This study reveals that walnut shell is an efficient and cost effective adsorbent for Cr(VI) removal and it can be a solution for Cr(VI) discharging industries.

- **Keywords:** Adsorption; Regeneration; Walnut shell; Breakthrough curve; Kinetic modelling

Tausif Ahmad, Chandan Guria, Ajay Mandal. *Synthesis, characterization and performance studies of mixed-matrix poly(vinyl chloride)-bentonite ultrafiltration membrane for the treatment of saline oily wastewater*. Pages 703-717.

The present study deals with the improvement of surface morphology, hydrophilicity and antifouling behavior of polyvinyl chloride (PVC) membrane by adding bentonite for ultrafiltration of oil-in-water emulsion under wide range of salinity (0–35000ppm). Flat-sheet UF membranes were prepared by phase inversion technique using N, N-dimethylacetamide (DMAc) and water. Viscoelastic properties of the membrane casting solution were measured to fix sonication frequency, membrane casting speed and casting solution composition. Field-emission-scanning-electron-microscope and atomic-force-microscope were used to measure surface-porosity, pore-size distribution, pore density and roughness parameters of the membranes. Hydrophilicity of the membranes was determined by measuring equilibrium water content, contact angle and work of adhesion, whereas antifouling character was quantified by flux recovery ratio using saline oily-wastewater. Casting solution with PVC:DMAc:bentonite=12.0:87.23:0.77 (i.e., PVC/bentonite-6) exhibited the maximum loss tangent and in-phase dynamic viscosity and resulted enhanced surface porosity (56.42–58.62%), root mean square surface roughness (127.6nm), surface pore density (42.29–32.05 pores μm−2), hydrophilicity (work-of-adhesion:111.08mNm−1) and antifouling character (flux-recovery-ratio:81.97%). PVC/bentonite-6 also delivered improved performance to separate oily-wastewater with zero salinity (oil rejection: 97.0% and permeate flux: 186Lm−2h−1) and 35000ppm salinity (oil rejection: 92.5% and permeate flux: 94nLm−2h−1) at 0.2MPa trans-membrane pressure.

- **Keywords:** Polyvinyl chloride; Bentonite nanoclay; Viscoelasticity; Saline oily-wastewater; Ultrafiltration

Chiara Vianello, Ernesto Salzano, Giuseppe Maschio. *Thermal behaviour of Peracetic Acid for the epoxydation of vegetable oils in the presence of catalyst*. Pages 718-726.

Peroxyacids are commonly used in chemical processing, synthesis and bleaching. Recently, they have been demonstrated to be very versatile for the epoxidation of unsaturated oil, aiming at the synthesis of polyepoxides (plasticizer, resins and adhesives). These processes are characterized by high yields and selectivity. However, due to their hazard and instability, the peroxy reactants are often obtained from the corresponding organic acid in situ by combination with Hydrogen Peroxide, in the presence of a mineral (Sulphuric or Phosphoric) acid as catalyst. The aim of this study is to analyse the thermal stability of the catalytic system used for vegetable oil peroxidation with the purpose of operating under safety conditions and then identify the safety parameters necessary to prevent the runaway reaction. This paper presents the study of the decomposition of peroxyacetic acid in aqueous phase by using a Thermal Screening Unit. Also, the effect of the presence of the acid catalysts was analysed.

- **Keywords:** Peracetic Acid; Decomposition; Runaway reaction; Thermal risk; Kinetic

A.M. Birk, F. Heymes, R. Eyssette, P. Lauret, L. Aprin, P. Slangen. *Near-field BLEVE overpressure effects: The shock start model*. Pages 727-736.

Abstract: This paper presents the results of a small scale experimental study of BLEVE overpressure effects. Testing consisted of a sealed aluminum tube (0.6L) filled with either water or propane, being heated by a flame until the internal pressure led to catastrophic failure and explosion. Three parameters were controlled during the experiments: the failing pressure, the weakened length on the tube and the fill level. BLEVEs were obtained with tests involving water and propane. Blast gages and optical techniques were used to characterize the shock wave escaping from the failing tube. The results obtained suggest that the lead shock was primarily generated by the vapor space. Overpressure results obtained were compared with the predictions of existing models and found to be in reasonable agreement except for overpressures measured vertically above the cylinder where the overpressures were highest. A prediction model based on only vapor space characteristics was developed. Images show that the shock was fully formed at some distance away from the vessel opening and this was due to the non-ideal opening of the vessel. The model developed was based on the characteristics of the shock when fully formed away from the tube. These characteristics were defined using a combination of imaging, pressure measurements, and predictions from shock tube theory.

- **Keywords:** BLEVE; Explosion; Blast overpressure; Shock initiation; Risk assessment

Min Hua, Xiaohui Shen, Juan Zhang, Xuhai Pan. *Protective water curtain ammonia absorption efficiency enhancement by inorganic and surfactant additives*. Pages 737-744.

Comparative tests with and without three inorganic salts (FeCl3, AlCl3 and MgCl2) and surfactants in water curtain were carried out experimentally to investigate the ammonia decontamination in confined space. Experimental scenarios include single additives of each inorganic salt and their pair combination of compound additives. The results show that the single inorganic salt can promote the chemical decontamination effect of water curtain on ammonia decontamination and the compound additives have better synergistic effect on ammonia decontamination. The decontamination mechanism consists of physical absorption, air entrainment, physical block and chemical absorption. The best optimal ratio of compound additive solution is 5:5.The addition of surfactant additive improves the surface properties of the solution, reduces the surface tension, increases the interface area between water curtain and ammonia, efficiently promotes the physical and chemical performances of contained inorganic salt additive. Moreover, the causticity of inorganic additives were tested and the results showed that the added inorganic salts hardly have corrosive effect on facilities. X-ray diffraction was also conducted to analyze the characteristics of water curtain decontamination products. The results indicates that the decontamination products are mainly chloride and hydroxide, which lead to no secondary pollution.

- **Keywords:** Water curtain; Ammonia decontamination; Compound additive; Synergistic effect; Optimal ratio

Ilyas Sellami, Rachid Nait-Said, Charles de Izarra, Khaled Chetehouna, Fatiha Zidani. *Quantitative consequence analysis using Sedov-Taylor blast wave model. Part I: Model description and validation*. Pages 763-770.

Abstract: BLEVE (Boiling Liquid Expanding Vapor Explosion) phenomenon is one of the major industrial accidents observed in gas processing industry, which remains a major concern for risk decision-makers. BLEVE blast wave mechanism has been widely studied by several authors who proposed simplified approaches based on simple physical models or empirical correlations, but only few approaches including analytical solutions have been undertaken. Moreover, the simplified and empirical approaches are not very satisfactory because they overestimate overpressure measures. In this paper (Part I), an analytical model based on Sedov-Taylor blast wave solution and self-similar theory, which is of great interest in various fields of physics, is proposed for estimating BLEVE overpressure effects. The parameters characterizing the blast wave evolution (overpressure, radius and velocity) are established by applying the Vashy-Buckingham theorem (Pi theorem). To demonstrate the ability of the proposed model to deliver reliable predictions, a validation with large and medium-scale BLEVE experiments issued from the literature is carried out. Furthermore, a comparison with the TNT equivalent model and other models (empirical and simplified physical) is performed. The results of these comparisons are very encouraging and show good agreement in terms of precision. This is Part I of two papers, focusing on description and validation of the Sedov-Taylor blast wave model. Part II deals with application of the model on a LPG accumulator in an Algerian gas processing unit.

- **Keywords:** Blast wave; BLEVE; Overpressure; Sedov-Taylor model; Self-similar theory

I. Sellami, R. Nait-Said, K. Chetehouna, C. de Izarra, F. Zidani. *Quantitative consequence analysis using Sedov-Taylor blast wave model. Part II: Case study in an Algerian gas industry*. Pages 771-779.

In the oil and gas industry, it is common to use gas liquefaction that allows storage and transport of large quantities of LNG and LPG. One of the main disadvantages of this storage mode is the BLEVE risk, which remains a major concern for risk decision-makers. In order to prevent the occurrence of this risk and reduce its impact, risk analysts often use quantitative risk analysis (QRA), which is based on the understanding and quantification of the accidental phenomena and their consequences (overpressure, thermal radiation, toxicity dose). QRA is a rigorous and advanced approach that requires reliable data in order to obtain a good estimate and control of risks. The main objective of this paper (Part II) is to integrate the Sedov-Taylor model developed in Part I into the QRA approach in order to evaluate BLEVE blast effect, and illustrate it with a case study on a pressurized LPG accumulator located in the MPP3-plant of SONATRACH company in the Hassi R'Mel gas field (the largest gas field in Algeria). A parametric analysis of the fuel mass, temperature at failure and rupture pressure is carried out to study their influence on the evolution of BLEVE overpressure. In addition, the evaluation of BLEVE thermal effect is performed in order to better realize an exhaustive QRA. Through this application, the results show the great relevance of the Sedov-Taylor model in the consequence analysis and also in the development of process safety recommendations.

- **Keywords:** Blast effect; BLEVE; Consequence analysis; QRA; Sedov-Taylor model

Chularat Sakdaronnarong, Wanvipa Pipathworapoom, Thanapon Vichitsrikamol, Teerawat Sema, Pattaraporn Posoknistakul, Wanida Koo-amornpattana, Navadol Laosiripojana. *Integrative process for a sugarcane bagasse biorefinery to produce glucose, bio-oil and carbon microspheres*. Pages 1-13.

Selective fractionation of cellulose from sugarcane bagasse (SCB) for the production of fermentable sugars was studied. The SCB was pretreated by hydrothermal pretreatment using five different types of solid acid catalysts (SACs): (1) self-synthesis SiO2–OSO3H,

(2) $SO_4^{2-}/TiO_2/Fe_3O_4/WO_3$, (3) sulfonated bentonite and commercial SAC, (4) Amberlyst® 15, and (5) Dowex® 50WX8. Fractionation of SCB was conducted in a combination with choline acetate (ChOAc) ionic liquid (IL) at moderate temperature. After enzyme hydrolysis, the highest total reducing sugar (TRS) yield of 78.1% was achieved when pretreated with $SiO_2–OSO_3H$. For the black liquor from fractionation, the highest amount of lignin could be precipitated from ChOAc IL through treatment with $SO_4^{2-}/TiO_2/Fe_3O_4/WO_3$. Pyrolysis of dry precipitated lignin was performed at 400 and 500°C under a nitrogen atmosphere, and phenolic-rich oil was produced. Carbon microspheres appeared in the solid phase from the pyrolysis. It was postulated that lignin was first degraded to phenol with an aromatic structure, while other sugar residues (C5 and C6) in the lignin molecule formed ring compounds. These compounds underwent condensation polymerization as a shell-like shape, and carbon rich microspheres were thus formed.

- **Keywords**: Solid acid catalyst; Ionic liquid; Sugarcane bagasse; Hydrothermal; Pyrolysis; Bio-oil; Carbon microspheres

Sangshan Peng, Xuemei Wu, Songlan Sun, Wanting Chen, Min Li, Jie Li, Gaohong He. *A morphology strategy to disentangle conductivity–selectivity dilemma in proton exchange membranes for vanadium flow batteries*. Pages 126-136.

A novel integrally thin skinned asymmetric proton exchange membrane (ITSA-PEM) is proposed to disentangle the typical conductivity–selectivity dilemma in PEMs for vanadium flow batteries (VFBs). The membrane is successfully fabricated by a porogen-leaching-out method. It consists of a porous sublayer and an ultrathin skin layer, which is defect-free verified by the high H_2/N_2 separation factor of 64.9. The degree of sulfonation (DS) of PEM is reduced to extremely low (DS=36.3%) to suppress swelling, and numerous interconnected pores are introduced to facilitate proton transfer. Low swelling ratio and defect-free skin layer lead to undetectable vanadium permeation. Meanwhile, the area resistance of ITSA-PEM is dramatically lowered to 2.1Ωcm2 from 5.4Ωcm2 of the dense PEM. Therefore a membrane with both improved proton conductivity and ion selectivity is obtained. Low DS also equips the membrane with sufficient mechanical strength and enhanced thermal stability. The VFB assembled with ITSA-PEM displays high energy efficiencies (EE: 75.6–90.2%) over a current density of 20–80mAcm−2, much superior to those of Nafion 211 (EE: 55.9–73.4%). It also shows favorable stability and slow capacity decay rate during cycling test over 50 cycles.

- **Keywords:** Defect-free skin layer; Asymmetric morphology; Conductivity–selectivity dilemma; Porogen-leaching-out method; Proton exchange membrane; Vanadium flow battery

Byung Wook Hwang, Jeong Hwan Lim, Ho Jin Chae, Ho-Jung Ryu, Doyeon Lee, Joong Beom Lee, Hana Kim, Soo Chool Lee, Jae Chang Kim. *CO_2 capture and regeneration properties of MgO-based sorbents promoted with alkali metal nitrates at high pressure for the sorption enhanced water gas shift proces*. Pages 219-227.

We investigated the CO_2 sorption and desorption properties of MgO-based sorbents at pressures ranging from 1 to 20atm. The effects of desorption gas composition on regeneration was also investigated, using temperature programmed desorption (TPD). The MgO-based sorbents promoted with alkali metal nitrate without K_2CO_3 had the highest CO_2 capture capacity and good regeneration properties, compared to MgO-based sorbents with both nitrates and K_2CO_3. Alkali metal nitrates play an important role in improving CO_2 capture capacity by providing channels for CO_2 diffusion. The addition of K_2CO_3 causes sorbent aggregation, resulting in their deactivation. Also, the necessary

regeneration temperature increased from 430°C to 650°C with an increase in the pressure and regeneration CO2 concentrations.

- **Keywords:** MgO; Nitrates; High pressure; SEWGS; CO2 capture; IGCC

Wei Tan, Chaojie Li, Kang Wang, Guorui Zhu, Yang Wang, Liyan Liu. *Dispersion of carbon dioxide plume in street canyons*. Pages 235-242.

When road tankers or pipelines fail in a city, the released gas generates cloud in street canyons. The toxic heavy gas cloud pollutes the environment and harms the living being's life. The concentration distribution and trail of the cloud are very important parameters for the emergency response. The wind tunnel experiment and the Computational Fluid Dynamics (CFD) method were applied in studying the transport and dispersion of carbon dioxide (CO2) plume, which was a typical type of heavy gas, in a long street with an intersection. The numerical simulated results using the SST k-ω model were in acceptable agreement with the experimental data. The stationary pre-release flow field in street canyons was characterized by the lee eddy generated on the sharp edges of the building top and sides. In this work, the entire releasing and dispersing process of CO2 can be divided into two stages or two regions. The motion of CO2 cloud was primarily determined by the jet speed and slightly affected by wind in near-source region. The next stage began with the collapse of CO2 cloud. The gravity and wind together influenced the concentration distribution of CO2. Both leakage rate and wind speed had significant impacts on CO2 distribution pattern within an urban street canyon.

- **Keywords:** Street canyon; Wind tunnel; CFD; Dispersion; Carbon dioxide; SST k-ω mode

Billie Yan Zhang Hiew, Lai Yee Lee, Xin Jiat Lee, Suchithra Thangalazhy-Gopakumar, Suyin Gan, Siew Shee Lim, Guan-Ting Pan, Thomas Chung-Kuang Yang, Wee Siong Chiu, Poi Sim Khiew. *Review on synthesis of 3D graphene-based configurations and their adsorption performance for hazardous water pollutants*. Pages 262-286.

Water pollution is a global health and environmental issue affecting all life forms. The treatment of water polluted by dyes, heavy metals and pharmaceuticals is a major challenge to operators of wastewater treatment facilities. Adsorption technology functions effectively in removing these pollutants using specific adsorbents. Graphene oxide (GO) and its three dimensional (3D) configurations are new carbon-based adsorbents. With superiorly large surface area, high porosity and large variety of functional groups, these materials have been tested for their potential application in wastewater treatment. This review focuses on the synthesis methods of 3D graphene-based structures and their adsorption performance of dyes, heavy metals and pharmaceuticals. Various synthesis methods have been successfully developed demonstrating the feasibility of configuring graphene into porous 3D networks. These methods can be categorised into direct synthesis and solution-based methods. The 3D graphene structures portrayed relatively high adsorption capacities for the three pollutant groups. Their adsorptive properties were influenced by characteristics of pollutant, adsorbent surface and process parameters. The major adsorption mechanisms of the 3D graphene-based structures were identified to be hydrogen bonding, electrostatic, π-π and hydrophobic interactions. This review indicated that 3D graphene configurations are promising solutions for practical application of carbon nanomaterials in wastewater treatment.

- **Keywords:** Graphene oxide; 3D graphene-based structures; Adsorption; Pharmaceuticals; Dyes; Heavy metals

Wei Tan, Kang Wang, Chaojie Li, Liyan Liu, Yang Wang, Guorui Zhu. *Experimental and numerical study on the dispersion of heavy gases in urban environments*. Pages 640-653.

Heavy gas dispersion, including gravity settling that causes longstanding high-concentration zones near the ground, has become a popular research topic in recent years. A series of wind tunnel experiments containing complex layouts of building blocks were carried out to illustrate the comprehensive effect of obstacles and environmental factors on heavy gas dispersion and distribution in urban environments. The factors of wind velocity and direction, temperature, and relative humidity were considered. Five stages of variations in the carbon dioxide concentration with respect to both, wind velocity and time, were investigated at specific positions in urban environments. This paper proposes a mathematical approach to describe the concentration increasing and decreasing stage with linear fit and polynomial fit, respectively. A critical wind velocity profile,V=1.26(y0.28)0.22, at which both, the growth rate and the maximum concentration, can be at their lowest near the source. Heavy gas accumulates obviously on streets that are perpendicular to the wind direction and can flow across the roof of buildings much more easily. Gas accumulation dangerous concentration may occur near the leeward side of building due to the low pressure effects. The influence of temperature and relative humidity was apparent mainly near the source. Meanwhile, computational fluid dynamics was used to simulate the effect of gravity settling and fluid field details. Simulation results with a realizable turbulence model were obtained to compare with the experimental data, while conservative results were obtained for the building roofs.

- **Keywords:** Heavy gas; Urban environment; Dispersion process; Wind tunnel experiments; Computational fluid dynamics simulation

Muflih A. Adnan, Sagir Adamu, Oki Muraza, Mohammad M. Hossain. *Fluidizable NiO–Fe2O3/SiO2–γAl2O3 for tar (toluene) conversion in biomass gasification*. Pages 754-762.

This communication reports synergetic effects of bimetallic Ni–Fe on NiO–Fe2O3/SiO2–γAl2O3 catalysts for biomass tar (toluene) conversion. The catalysts were successfully synthesized using a one-pot, solvent-deficient method and characterized using XRD, N2 adsorption isotherm and NH3-TPD techniques. The introduction of SiO2 enhanced thermal stability of the NiO–Fe2O3/SiO2–γAl2O3 catalysts, as observed in XRD and BET surface area analysis. The synthesized NiO–Fe2O3/SiO2–γAl2O3 catalysts showed high BET specific surface area (52–58m2/g) even after calcination at 950°C. The NH3-TPD analysis exhibited that the addition of NiO significantly decreased the strong acid sites of the NiO–Fe2O3/SiO2–γAl2O3 catalysts. The performance of the synthesized catalysts were evaluated in a fluidized CREC Riser Simulator using toluene as a tar model compound. The NiO containing NiO–Fe2O3/SiO2–γAl2O3 catalyst yielded high toluene conversion with higher H2 concentration in the produced gas, as compared to Fe2O3/SiO2–γAl2O3 catalyst. The presence of nickel promoted both methane reforming and water-gas shift reactions, contributed to higher H2 concentration in the producer gas. A gasification process model, as developed in Aspen Plus, also showed that hydrogen composition of the producer gas can also be enhanced by adjusting the gasification temperature, pressure and steam/biomass ratios. These results indicate that the NiO–Fe2O3/SiO2–γAl2O3 catalyst has a great potential for industrial use since it is a relatively cheap, less toxic, and stable for extended period of gasification operation. The spent catalyst materials are also useful to produce other commercial products, such as Portland cement and glass-ceramics.

- **Keywords:** Fluidized bed; Biomass; Gasification; Tar (toluene) conversion; Bimetal oxide catalyst; Silica–alumina

Kit Wayne Chew, Shir Reen Chia, Yee Jiun Yap, Tau Chuan Ling, Yang Tao, Pau Loke Show. *Densification of food waste compost: Effects of moisture content and dairy powder waste additives on pellet quality*. Pages 780-786.

Densification of food waste compost through pelletizing is essential to increase the bulk density, expand its storability, provide ease of transportation, as well as to enable easier handling of the compost. Compost in its natural form takes up a lot of space and has a high powder dispersion rate which makes it less safe and difficult to handle. The compression of these composts into pellet forms will reduce the managing issues associated with the natural compost feedstock. In this study, the pelletizing of food waste compost by adjusting the moisture content and dairy powder waste addition was performed to evaluate the pelletization performance. The physical and mechanical properties such as moisture content, bulk density, producibility, particle density, compressive strength and moisture resistance were evaluated for the pelletized compost products. This research indicates that the addition of dairy powder additives containing lactose is very beneficial in improving the pellet production rate as well as the properties of the pellets. The pellets with lactose addition showed better producibility, better compressive strength and higher density. The presence of more solid bridges was also observed with the addition of lactose additives which crystallize and lead to stronger bonds within the pellet.

- **Keywords:** Compost pellet; Food waste compost; Lactose additive; Moisture content; Pelletization

Malin Song, Shuhong Wang. *Measuring environment-biased technological progress considering energy saving and emission reduction*. Pages 745-753.

This study proposes a mathematical definition of environment-biased technological progress that can evaluate energy saving and emission reduction abilities. Further, it proposes the concepts of absoluteness and relativity, while extending the classical non-radial slack-based measure in order to establish an advanced slack-based measure model. In addition, a super-efficiency advanced slack-based measure model is set up to test the effectiveness and growth rate of environment-biased technological progress in China. Finally, with China entering a new normal since 2012, economic growth data for 1890 coal production enterprises for 2012–2014 are collected to measure the conditions of environment-biased technological progress in each location and registration type. The results indicate that, compared to existing methods, the proposed method is useful and universally applicable.

- **Keywords:** Biased technological change; Slack-based measure; Non-radial; Energy saving; Emission reduction; Implications for industry 4.0