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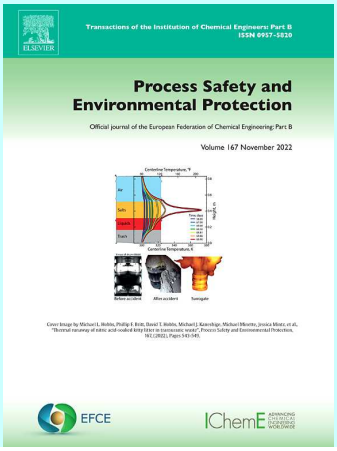

V. Vasanthakumar, Murad Alsawalha, Thamer Alomayri, Saud Allehyani, Yi-bo Hu, Ming-Lai Fu, Baoling Yuan. *α-Bi2(MoO4)3 nanorods decorated with two-dimensional g-C3N4 nanosheets for efficient degradation of doxycycline under visible light illumination*. Pages 1-13.

Water pollution caused by pharmaceutical and personal care products (PPCPs) has been significant stress on the water management system. The development of effective and recyclable material for PPCPs removal has become essential. In the present work, a highly efficient g-C3N4/α-Bi2(MoO4)3 nanocomposites was prepared by a simple wet impregnation method and investigated as a catalyst for the photocatalytic degradation of doxycycline under visible light irradiation. The as-prepared catalysts with various mass ratios were systematically characterized with XRD, FT-IR, UV−vis, FE-SEM, EDX, FE-TEM, and XPS. The equal weight ratio (50:50) of g-C3N4/α-Bi2(MoO4)3 nanocomposite exhibits excellent visible light absorption and outstanding doxycycline photodegradation due to the improved separation efficiency of photo-generated charge carriers. After four consecutive cycles, the equal weight ratio (50:50) of g-C3N4/α-Bi2(MoO4)3 nanocomposite shows superior photostability. The scavenger study was carried out to investigate the role of active species in photodegradation activity. More superoxide radicals present on the surface of g-C3N4/α-Bi2(MoO4)3 nanocomposites can significantly enhance the photocatalytic performance. Therefore, a simple wet impregnation method was used to produce a low-cost g-C3N4/α-Bi2(MoO4)3 photocatalyst with the influential effects of removing pharmaceutical contaminants in water bodies.

- **Keywords:** G-C3N4/α-Bi2(MoO4)3 nanocomposites; Doxycycline; Photocatalyst; Visible-light photocatalyst

Fernanda Paludetto Pelaquim, Raphaela Gabrí Bitencourt, Antonio Marinho Barbosa Neto, Irede Angela Lucini Dalmolin, Mariana Conceição da Costa. *Carbon dioxide solubility in Deep Eutectic Solvents: Modelling using Cubic Plus Association and Peng-Robinson equations of state*. Pages 14-26.

Carbon Dioxide (CO2) is the greenhouse gas that most contributes to global warming and climate change due to fossil fuels combustion, transportation, and other industrial process. Carbon capture, storage, and utilization (CCSU) is an effective method to reduce CO2 emission. Chemical absorption is the most straightforward technology for post-combustion CO2, and monoethanolamine (MEA) has been proved to be the most efficient chemical solvent. However, MEA is not environment friend, thus indicating the need for developing eco-friendly absorbers for CO2 capture, such as Deep Eutectic Solvents (DESs). Despite recent experimental studies investigating CO2 solubility in DESs, thermodynamic modelling is important to understand the system behavior. Thus, this study modelled CO2 solubility in thirteen DESs found in a large range of temperature (from 303.15 to 343.15 K) and pressure range (from 0.06 to 12 MPa). Cubic-Plus Association (CPA) and Peng-Robinson 78 equations of state were used to compare efficiency. The results indicate that fitting the binary interaction parameter (kij) promotes a better reproduction result than considering kij equals zero. Despite all association schemes of CO2 providing accurate results, the 4 C association scheme (two electron acceptors and two electron donors) resulted in better equilibrium description. Both models describe experimental data very well, yet the individual component approach presents better results than pseudo-component approach, corroborating with DESs definition.

- **Keywords:** Carbon Dioxide; Carbon capture, storage, and utilization; Deep Eutectic Solvents; Cubic-Plus Association; CO2 solubility

Dong Xu, Jun Li, Jun Liu, Xinghong Qu, Hailing Ma. *Advances in continuous flow aerobic granular sludge: A review*. Pages 27-35.

Aerobic granule in continuous-flow process is drawing increasing global interest in a quest for an efficient and innovative technology in the biological wastewater treatment. This paper presents a review of the literature on the development of extended treatments for complicated pollutants, numerous configurations of continuous flow aerobic granular reactors and enhancements of granule stability in long-term operation. The challenges and prospects of full-scale applications of this process were discussed. The review attempted to shed light on our growing knowledge to this technology, which may accelerate the spread of practical applications.

- **Keywords:** Aerobic granular sludge (AGS); Continuous flow; Sequencing batch reactor (SBR); Stability; Full-scale

Mojtaba Mehdinia Lichaei, Farhang Pazani, Abdolreza Aroujalian, Denis Rodrigue. *Two-step surface functionalization/alignment strategy to improve CO2/N2 separation from mixed matrix membranes based on PEBAX and graphene oxide*. Pages 36-47.

In this study, a simple method to prepare mixed matrix membranes (MMM) based on Pebax with functionalized/oriented graphene oxide (GO) nanosheets is presented to improve CO2/N2 separation. First, the GO nanosheets were surface modified with different amounts of m-phenylenediamine (mPD) to maximize the CO2 adsorption affinity and minimize GO agglomeration within the matrix. Then, an external electric field was applied to organize/orient the GO nanosheets (modified and unmodified) during membrane preparation. The separation performance results showed that the CO2

permeability of unmodified and amine-functionalized GO-filled MMM respectively increased by 1.7 and 2.1 times compared to the neat matrix. This improvement is attributed to the high affinity of amino groups for CO2 uptake. Furthermore, applying a vertical electric field increased the CO2 permeability compared to a random GO orientation state by 1.3 and 2.8 times for the unmodified and modified GO-filled MMM, respectively. This significant improvement is related to a lower tortuosity in the membrane, improving the passage of gas molecules. Overall, the combination of surface treatment (amino group) and orientation (electric field) on GO nanosheets leads to better CO2 permselectivity for the membranes studied.

- **Keywords:** Gas separation; Mixed matrix membranes; Pebax; Aminated graphene oxide; Aligned graphene oxide

Jing Zhang, Yanling Zhao, Siqi Wu, Guangchao Jia, Xin Cui, Peitao Zhao, Yimin Li. *Enhanced adsorption of malachite green on hydroxyl functionalized coal: Behaviors and mechanisms*. Pages 48-57.

The discharge of untreated colored wastewater poses a severe threat to global health. This work reports a simple yet highly efficient way to modify Zhundong coal (MZD) with hydroxyl functional groups for malachite green (MG) removal. The modification significantly improved the adsorption capacity of MG from 63.0 mg/g to 538.7 mg/g. According to Fourier transform infrared spectroscopy, zeta-potential analyzer, X-ray photoelectron spectroscopy, and N2 absorption characterization, the improvement in adsorption capacity was mainly attributed to the enhancement of hydroxyl functional groups on the surface of coal. The adsorption of MG on MZD depended on pH, and the highest removal efficiency reached 99.7% at pH 10 with an initial MG concentration of 500 mg/L. The adsorption process was mainly controlled by chemisorption, and it was endothermic and spontaneous according to thermodynamic analysis. The adsorption data could be well reproduced by the pseudo-second order kinetic model and the Redlich-Peterson isotherm model. The MZD shows good regeneration performance with only a 16.9% reduction of initial adsorption capacity after five circles. Hydrophobic interactions, π-π interactions, and pore-filling contributed to adsorption, whereas electrostatic interactions played a dominant role in the MG removal by MZD. This work provides a new sight to prepare useful and cheap adsorbents from coal to remove contaminants from printing and dyeing wastewater.

- **Keywords:** Malachite green; Zhundong coal; Hydroxyl functional groups; Adsorption; Electrostatic interactions

Fitri Widhiastuti, Linhua Fan, Jorge Paz-Ferreiro, Ken Chiang. *Oxidative degradation of bisphenol A in municipal wastewater reverse osmosis concentrate (ROC) using ferrate(VI)/hydrogen peroxide*. Pages 58-67.

The combination of ferrate(VI) with hydrogen peroxide (H2O2) was used for the degradation of bisphenol A (BPA) spiked in municipal wastewater reverse osmosis concentrate (ROC). The results showed that the combined Fe(VI) and H2O2 oxidant provided an additive effect to achieve greater degradation efficiencies of BPA in ROC compared to the use of Fe(VI) or H2O2 alone. The degradation efficiency of BPA was studied in detail by assessing the operating conditions, including Fe(VI) dosage, H2O2 dosage, the dosing strategy of Fe(VI) and H2O2, solution pH, and the initial concentration of BPA. It was found that over 99.0% of BPA was degraded (50 μg L^{-1}) by using [Fe(VI)]/[H2O2] at a ratio of 1050:5000 and at pH 8.0. In addition, the degradation was also accompanied by 37.2% of dissolved organic carbon (DOC) removal and 94.0% of UV254 reduction. However, when the excess amount of H2O2 was added, it was found that H2O2 started to inhibit the degradation and the degradation efficiency of BPA in ROC lowered. It was also found that the simultaneous addition of Fe(VI) and H2O2 provided satisfactory BPA degradation. Similar degradation efficiency could be

achieved by injecting the second oxidant into the system 10 min after adding the first oxidant at time zero. The apparent second-order reaction rate constant (kapp) obtained was 67.9 × 103 M−1 s−1 at a [Fe(VI)]/[H2O2] ratio of 1050:5000. The overall ecotoxicity of the treated water samples as measured by the Microtox bioassay technique decreased after the Fe(VI)/H2O2 treatment, which indicated that an insignificant amount, if not none, toxic degradation by-products was formed by the oxidative action of the Fe(VI)/H2O2 combined oxidant. The use of Fe(VI)/H2O2 as an alternative treatment option of cost-effectiveness than Fe(VI) alone in water and wastewater industries.

- **Keywords:** Bisphenol A; Ferrate(VI)/H2O2; Oxidative degradation; Kinetics; Reverse osmosis concentrate

Arun Kumar, Monika, Ranjeet Kumar Mishra, Saurabh jaglan. *Pyrolysis of low-value waste miscanthus grass: Physicochemical characterization, pyrolysis kinetics, and characterization of pyrolytic end products*. Pages 68-81.

The current study explored the bioenergy potential of waste miscanthus grass (WMG). The kinetic study of WMG was evaluated via two model-free methods, in a thermogravimetric analyzer (TGA), at dynamic heating rates under an inert ambiance. The pyrolysis was performed in a semi-batch fixed bed reactor at 500 oC, 80 oC min heating rate, and 1 mm particle size. The evolution of hot vapours during pyrolysis was explored using a TGA-FTIR analyzer. Finally, the bio-oil and biochar were characterized by their physicochemical properties. The kinetic results established that WMG followed a multi-step decomposition process, and the average activation energy gained from KAS and ST was found to be 197.66 and 179.64 kJ mol-1, respectively. TGA-FTIR study revealed the foremost release of carbon dioxide (28.22%), followed by a carbonyl (25.40%), and ether (19.12%). Further, the pyrolysis of WMG yielded 29.32 wt% of bio-oil at the optimized condition whereas, physicochemical results of bio-oil established; 65.16% carbon content, 26.16 MJ kg-1 HHV, 34.15 cP viscosity, and 812 kg m-3 density. GC-MS study of bio-oil confirmed the maximal release of hydrocarbons and phenols. Finally, characterization results of miscanthus grass biochar (MGB) demonstrated an excellent feedstock for industrial and domestic applications.

- **Keywords:** Low-value waste biomass; Kinetics study; Bio-oil; Pyrolysis; Model-free methods; Activation energy; Biochar

Bhushan Pawar, Mitchell Huffman, Faisal Khan, Qingsheng Wang. *Resilience assessment framework for fast response process systems*. Pages 82-93.

Resilience is essential to ensure safe and sustainable process operations. It plays a critical role in enabling operations in the remote and extreme environments encountered during operations held offshore or in the Arctic. Resilience is a property of the process or system, and considers three distinct characteristics: absorption, adaptation, and recovery. This work proposes a resilience assessment framework of process systems with fast responses, such as reaction systems. The three characteristics are modelled using system design variables with covariate consideration. Subsequently, these three characteristics are integrated to assess resilience. To enhance the resilience, design changes and operational interventions are explored. The proposed framework is explained using the assessment of an autocatalytic reactor as a case study. A thermal runaway reaction is modelled for resilience, and operational intervention strategy such as adding inhibition is tested to enhance the resilience of the reactor. It was concluded that as the inhibitor injection time was decreased from 5.8 min to 1 min, the value of the proposed resilience metric increased from 0.7 to 0.9. This case study confirms the applicability and effectiveness of the proposed framework.

- **Keywords:** Resilience; Reliability and maintainability; Chemical process systems; Mathematical modeling

Zhanguang Wang, Xiaoqin Zhang, Jinpeng Guo, Caifeng Hao, Yongming Feng. *Particle emissions from a marine diesel engine burning two kinds of sulphur diesel oils with an EGR & scrubber system: Size, number & mass*. Pages 94-104.

IMO has pushed out strict regulations to limit marine diesel engine emissions. EGR is a mature measure to reduce NOx emissions which would lead PM emissions risen. In this paper, An EGR system combined with a scrubber was built on a marine diesel engine. Based on the experimental platform, the characteristics of PM emissions were studied when the engine burning two kinds of sulfur diesel oils. The results showed that the particle size concentration curves show multimodal distribution and the average particle sizes increased. Most of the PM emissions were distributed in the nuclear mode interval. Moreover, EGR scrubber had a significant effect on removing PM with an efficiency of over 98% and the weighted value of PM emissions was 22.136 mg / kWh, which met China's first and second-stage emission regulations and US EPA Tier 4 emission regulations.

- **Keywords:** Marine diesel engine; EGR system; Sulfur diesel fuel; PM

Yu-Chen Chang, Yen-Ping Peng, Ku-Fan Chen, Ting-Yu Chen, Chen-Ting Tang. *The effect of different in situ chemical oxidation (ISCO) technologies on the survival of indigenous microbes and the remediation of petroleum hydrocarbon-contaminated soil*. Pages 105-115.

This study determines the effect of different in situ chemical oxidation (ISCO) technologies on soil microorganisms and total petroleum hydrocarbon (TPH) degradation. Permanganate is a moderate oxidant to the intrinsic microbes while persulfate causes severe bacterial death. TPH removal in the persulfate and permanganate systems is similar, which is higher than that in the hydrogen peroxide system. Permanganate is the most suitable oxidant for ISCO, followed by in situ bioremediation because of its persistence and low toxicity. Chemical oxidation dominates the removal of TPH throughout the experiment in the persulfate systems and during the initial stage in the hydrogen peroxide and permanganate systems. The toxicity of different catalysis/activation methods to in situ microbes decreases in the order: heat> Fe2+/citric acid> Fe2+>no catalysis/activation. If ferrous iron or citric acid is used to catalyze hydrogen peroxide, the pH must be controlled to prevent severe damage to the microbes. There is more dissolved organic carbon in solution in oxidation systems, which shows that the addition of an oxidant increases the solubility and bioavailability of the contaminant. Petroleum degraders are present in the contaminated soil and the addition of oxidants changes indigenous bacterial communities significantly.

- **Keywords:** Diesel; Oxidant; In situ chemical oxidation (ISCO); In situ bioremediation (ISB); Microbial community

Fang Xu, Wei Liu, Shi Bu, Lin Zhang, Jiamei Fang, Zhikang Yu, Weigang Xu, Hong Ding, Guangtian Huo. *Manufacturing non-sintered ceramsite from incinerated municipal solid waste ash (IMSWA): Production and performance*. Pages 116-130.

The resource utilization of solid wastes has become a critical problem in resource recovery. In this study, IMSWA (Incinerated municipal solid waste ash) was washed to remove chloride and then mixed with OPC (Ordinary Portland Cement) and SS (Silica Sol) to prepare a non-sintered ceramsite. Through single factor experiments, the quality

scores of water-washed IMSWA: OPC: SS is initially determined to be 6:3:1, and the curing time is 14 d. Then the uniform test design was used to optimize the ceramsite formula and the influence of different raw material ratios on the performance of the non-sintered ceramsite. Finally, use DPS (Data Processing System) optimization to determine the best raw material quality scores: 59% for IMSWA, 30% for OPC, and 11% for SS. The performance follows (1) Ceramsite's compact surface structure, ensuring high strength and low water absorption. (2) Ceramsite section forms a complex calcium aluminate hydrate gel (C-A-H) structure (3) A profit of $60.97/ton of ceramsite has good economic benefits. These findings demonstrate that preparing a non-sintered ceramsite with IMSWA is a promising artificial lightweight aggregate.

- **Keywords:** Non-sintered ceramsite; IMSWA (Incinerated Municipal Solid Waste Ash); Product performance; Production efficiency

Kuibin Zhou, Mengya Zhou, Mengyuan Huang, Yifan Wang. *An experimental study of jet fires in pits*. Pages 131-143.

The explosion of underground pipelines could cause a big crater in which a gas leakage occurs to induce a large jet fire. The pit wall would significantly affect the leaked gas flow and the subsequent jet fire behavior. This paper presents a systematical investigation on such jet fire in a pit (JFP). A facility consisting of a jet fire apparatus and a rectangular pit, was designed for the experimental study. Phenomenon observation shows that the JFP can be divided into the impinging jet flame (IJF), transitive jet flame (TJF) and jet flame ejected from the pit top (JFEPT), due to the variation of the mode of air entrained into the pit with the nozzle exit velocity. A dimensionless heat release rate (HRR) coupling the pit geometrical property is developed to correlate the flame area in different pits, which clarifies the critical dimensionless HRR to distinguish the IJF, TJF and JFEPT. Using the dimensionless HRR, data fitting can well develop the correlation for the flame length of TJF and JFEPT, and the correlation is well validated by the small-scale and full-scale jet fires in irregular cuboid pits. The dimensionless HRR also can be used to well correlate the flame width. The radiative fraction of IJF still follows the law of the Froude number at the nozzle exit, while that of JFEPT should be predicted using the Froude number at the top opening of pit. As indicated by the variations of air entrainment mode and radiative fraction, the flame buoyancy gradually plays a more significant role than the nozzle exit momentum in the flame behavior, as the nozzle exit velocity increases to cause the evolution of JFP from IJF to JFEPT. In addition, a line source radiation model and two solid radiation models are proposed to predict the thermal radiation of JFP.

- **Keywords:** Jet fire; Pit; Flame length; Thermal radiation; Air entrainment

Meng Gu, Xiaodong Ling, Hanxiang Wang, Wenyi Dang, Xiao Teng, Anfeng Yu. *Experimental investigation into dynamic mechanical properties and explosion responses of polyurea elastomer*. Pages 144-157.

To reduce the threat of explosions to personnel safety, it can be considered to retrofit the existing buildings in high-risk areas of process industry in an economical and effective way. The mechanical behaviors of two types of polyureas were studied through a series of laboratory tests and field gas explosion tests, and the full-field explosion responses of polyurea were measured by a high-speed, three-dimensional digital image correlation (DIC) technique. It was found that polyurea exhibited a significant strain-rate-hardening effect, and the fracture strain of polyurea decreased significantly with the increase of strain rate. The failure criterion of the polyurea-coated fiber-reinforced cement board (FRCB) under gas explosion load conformed to the overpressure criterion. Polyurea could significantly improve the explosion resistance of the FRCB, and the reinforcement ability could be further improved by increasing the polyurea thickness of the rear face and strengthening on both sides. Dynamic thermodynamic and microscopic observations

revealed that under gas explosions, the polyurea was in the rubber–glass transition zone, which was beneficial for improving the ability of the material to attenuate shock waves.

- **Keywords:** Polyurea; Gas explosion; Strain rate effect; Digital image correlation; Glass transition

Lionel Nguemna Tayou, Roberto Lauri, Emma Incocciati, Biancamaria Pietrangeli, Mauro Majone, Federico Micolucci, Marco Gottardo, Francesco Valentino. *Acidogenic fermentation of food waste and sewage sludge mixture: Effect of operating parameters on process performance and safety aspects*. Pages 158-166.

The production of added-value bio-products and energy from waste streams while minimizing environmental impacts is a crucial aspect within the circular economy's principles. The biorefinery can be an exit to the constant increasing of organic food waste and sewage sludge to solve the issues of waste disposal. This work deals with the production of volatile fatty acids (VFA) as added-value products from food waste and sewage sludge mixture in a pilot scale acidogenic fermentation process. Moreover, due to the lack of information about safety aspects in the literature, the explosive risk of the fermenter has been assessed by means of the quantification of lower flammability limit (LFL) of the generated flammable gases. Different temperature and feedstock's composition were tested, as well as the effect of thermal hydrolysis. Mesophilic fermentation (37 °C) on thermally hydrolysed feedstock (48 h at 72 °C) ensured stability in terms of VFA production at high concentration (30 ± 2 gCODVFA/L) and CODVFA/CODSOL ratio (0.86 ± 0.09). Such condition also showed high LFL (28.9%), corresponding to a less hazardous condition compared to the other investigated, especially the thermophilic ones where LFL changed between 18% and 26%.

- **Keywords:** Acidogenic fermentation; Volatile fatty acids (VFA); Organic waste; Explosion risk; Lower flammability Limit; Flammable mixture gases

Jiuping Xu, Jiaxin Jiang, Yi Shi. *An innovative optimization model for sustainable hazardous waste reverse logistics network considering co-processing in cement kilns technology*. Pages 167-190.

As the rapid growth in hazardous waste (HW) is threatening both the environment and public health, more efficient disposal methods are needed. This paper proposes an innovative HW reverse logistics network (RLN) considering advanced co-processing in cement kiln technology, establishing three disposal lines to reduce HW volumes, develop renewable products, reduce greenhouse gas emissions, and conserve resources. To optimise the HW disposal process, a multi-objective optimisation model comprehensively considering social, economic, and environmental dimensions is proposed. Then a numerical example is used to demonstrated the validity of the proposed model and a real-world case is conducted to demonstrate the practicality and efficiency of the proposed model in determining the most suitable hazardous waste disposal facilities, transportation routes and transportation quantities. Scenario analyses under different decision-maker attitudes towards the objectives are conducted while also considering the influence of governmental disposal subsidies. Finally, practical policy suggestions are provided to guide scientific and sustainable HW disposal. This study concludes that 1) different decision maker and disposal subsidy levels affect the optimal system decisions, 2) advanced co-processing in cement kiln technology increases the effectiveness of the HW-RLN in terms of economic and environmental perspectives, and 3) policy subsidy support could encourage the application of co-processing in cement kiln technology; a unit disposal subsidy of 160 CNY is considered suitable for "technologically pessimistic" decision-makers, while 200–220 CNY is considered suitable for "technologically optimistic" decision-makers.

- **Keywords:** Hazardous waste; Reverse logistics network; Cement kilns; Sustainable disposal; Subsidy policy; Multi-objective optimisation

Guillaume Fayet, Annett Knorr, Patricia Rotureau. *First QSPR models to predict the thermal stability of potential self-reactive substances*. Pages 191-199.

Self-reactive substances are unstable chemical substances which can easily decompose and may lead to explosion in transport, storage, or process situations. For this reason, their thermal stability properties are required to assess possible process safety issues and for classification purpose. In this study, the first quantitative structure–property relationships (QSPR) dedicated to this class of compounds were developed to predict the heat of decomposition of possible self-reactive substances from their molecular structures. The database used to develop and validate the models was issued from a dedicated experimental campaign on 50 samples using differential scanning calorimetry in homogeneous experimental conditions. QSPR models were derived using the GA-MLR methods (using a genetic algorithm and multi-linear regressions) using molecular descriptors calculated by Dragon software based on two types of inputs: 3D molecular structures determined using the density functional theory (DFT), allowing access to three-dimensional descriptors, and from SMILES codes, favoring the access to simpler models, requiring no preliminary quantum chemical calculations. All models respected the OECD validation guidelines for regulatory acceptability of QSPR models. They were tested by internal and external validation tests and their applicability domains were defined and analyzed.

- **Keywords:** Quantitative structure-property relationships; Self-reactive substances; Thermal stability; Genetic algorithm

C.M.Vineeth Kumar, V. Karthick, D. Inbakandan, V. Ganesh Kumar, Eldon R. Rene, T. Stalin Dhas, M. Ravi, P. Sowmiya, C.G. Anjali Das. *Effect of selenium nanoparticles induced toxicity on the marine diatom Chaetoceros gracilis*. Pages 200-209.

Discharge of nanomaterials into the environment contributes to a diverse group of pollutants. In the present study, the toxicity of selenium nanoparticles (SeNPs) on the marine diatom Chaetoceros gracilis was studied in the laboratory by conducting 96 h toxicity experiments. The SeNPs were synthesized by reducing sodium selenite using L-cysteine and characterized by spectroscopic and microscopic techniques. X-ray photoelectron spectroscopic (XPS) data showed a distinctive selenide peak at 56 eV, indicating the oxidation states Se3d3/2 and Se3d5/2. Raman spectra results indicated the characteristic A1 and S mode of selenium (Se). Growth inhibitory experiments were performed (LC50 14.63 mg/L) for 96 h using various concentrations of SeNPs and its membrane damage to cells was observed. Upon treatment with SeNPs, an increased percentage of reactive oxygen species (ROS) production was detected from 28.77±3.13% to 130.55±3.16% after 96 h. Malonaldehyde (MDA), a biomarker of lipid peroxidation was quantified and exposure to 50 mg/L of SeNPs significantly ($p < 0.05$) increased MDA concentration from 4.31±0.02 to 5.05±0.05 μM in 96 h. The morphological distortion, including cell wall damage, that affects the cellular integrity upon exposure to SeNPs was evident from microscopic studies. These results clearly indicate that, even at lower concentrations, SeNPs toxicity on lower trophic organisms is significant enough to cause cellular level alterations.

- **Keywords:** Selenium nanoparticles; Chaetoceros gracilis; XPS; Flow cytometry; Reactive oxygen species; CLSM

Xiao Liu, Sen Yang, Tingjuan Feng, Huiyuan Zhong, Suqing Cao, Yanhua Chen. *Removal of amoxicillin from water by concrete-based hydrotalcites: Efficiency and mechanism*. Pages 210-217.

Amoxicillin (AMX) is a widely used broad-spectrum antibiotic whose presence in the environment has been widely concerned. In this work, two kinds of concrete-based hydrotalcites, C-LDH and Fe2+-C-LDH, were synthesized to remove AMX. C-LDH was used to adsorb AMX while Fe2+-C-LDH was employed to activate potassium persulfate (PDS) to degrade AMX. The adsorption characteristics of C-LDH for AMX were investigated, and the formula of Fe2+-C-LDH-PDS system was optimized. The removing mechanisms of AMX removal by C-LDH and Fe2+-C-LDH-PDS system were analyzed. C-LDH showed good performance for AMX adsorption as initial pH between 3–5, with maximum adsorption capacity of 49.7 mg/g. The C-LDH adsorbent could be regenerated by Na2CO3 elution. Fe2+-C-LDH exhibited good activity on PDS activation for AMX degradation, and could be used repeatedly. The optimum mass ratio of Fe2+-C-LDH to PDS was 2.6. C-LDH removed AMX through the electrostatic interaction and hydrogen bonding, while Fe2+-C-LDH-PDS degraded AMX by radical reaction. Concrete-based hydrotalcites illuminate a cheap and sustainable way for the removal of antibiotics.

- **Keywords:** Concrete based hydrotalcites; Antibiotics; Adsorption; Persulfate; Regeneration

A. Alcazar-Ruiz, L. Sanchez-Silva, F. Dorado. *Enhancement of BTX production via catalytic fast pyrolysis of almond shell, olive pomace with polyvinyl chloride mixtures*. Pages 218-226.

This work addresses enhanced benzene, toluene and xylene (BTX) production by catalytic fast co-pyrolysis from agroindustrial biomass blended with PVC and the use of prepared NaZSM-5 and HZSM-5. Results from catalytic fast pyrolysis of biomass indicates that oxygen-containing compounds decreased whereas aromatics increased. The catalytic effect of mineral content altered the co-pyrolysis intermediates by increasing the formation of mono-aromatics while reducing poly-aromatic hydrocarbons. Furthermore, the addition of PVC strongly influenced thermal decomposition of agricultural waste biomass, where BTX yields were enhanced up to 26.6% and 25.1% for 1:2 OP/PVC-HZ and 1:2 AS/PVC-HZ, respectively. Yields of toluene and xylene peaked at 19% and 10.5% hydrocarbon yields with 1:2 OP/PVC-HZ blend. Additionally, from the pyrolytic gas, CH4 yields increased while the CO2 yield fell due to oxygen removal by decarboxylation. These findings could provide a great insight into the olive pomace and almond shell valorization through an inexpensive and straightforward easy process.

- **Keywords:** Agroindustrial biomass residues; Polyvinyl chloride; Catalytic fast co-pyrolysis; Aromatics; BTX enhancement

P. Tamizhdurai, N. Sakthipriya, K. Sivagami, Bokam Rajasekhar, Indumathi M. Nambi. *Field studies on monitoring the marine oil spill bioremediation site in Chennai*. Pages 227-235.

Oil spills have become a threat to the ecosystem by releasing the petroleum hydrocarbons and gained substantial public concern in the Chennai coast. This study assesses the effectiveness of bioremediation and its impact on the environment due to remedial operations in the site. Soil and water samples were collected from the bio remediation site at regular intervals of the pit from the topsoil and 20 cm below the ground level from June 2017 to Nov 2019. The average TPH concentration present in the bottom and top soil of bioremediation pit were vary in the range of 21,238.4–46,600 mg/kg and 17577–26910 mg/kg. Central Pollution Control Board (CPCB) allowable limit for TPH concentration present in the soil should be 5000 mg/kg. We have

also observed that the mixing was not uniform in the pit and major amount of oil has been penetrated deep inside the soil. Results on gravimetric analysis showed that there was still a large amount of untreated long-chain hydrocarbons are there in the pit. From the results, we can conclude that nC30-nC40 and lower carbon range alkane intermediates have to be treated with additional treatment like thermal smoldering and pyrolysis.

- **Keywords:** Petroleum hydrocarbons; Bioremediation; Gravimetric analysis; Microbial growth

Fuyi Cui, Fuhai Liu, Yijie Tong, Shifeng Wang, Weigang Guo, Tianlong Han, Xudong Qiu. *Energy and exergy assessment of evacuated tube solar collector using water, Fe3O4 nanofluid and Fe3O4/MWCNT hybrid nanofluid*. Pages 236-243.

Environmental pollution has been intensifying in many countries because of the consistent misuse of fossil fuels. It's necessary to develop and utilize sources of solar energy. The main method to use solar energy is through the use of a solar collector. This paper aims to enhance and compare the thermal efficiency of solar collector by applying water, Fe3O4 nanofluid and Fe3O4/MWCNT hybrid nanofluid as the working fluids. The energy efficiency, exergy efficiency,exergy destruction and entropy generation were compared in this study. The evacuated tube solar collector shown the maximum efficiency when the Fe3O4/MWCNT hybrid nanofluid with mixing ration of 1/4 was used as the working fluid which was 26.4% higher than cases of the water. In addition, the exergy efficiency of the evacuated tube solar collector using 0.1 wt% Fe3O4/MWCNT hybrid(1:4) nanofluid and 0.1 wt% Fe3O4 nanofluid was improved by 55.2% and 42.1% comparing to the water, the maximum exergy efficiency was observed when Fe3O4/MWCNT(1:4) hybrid nanofluid was used. Water shown the highest entropy generation while Fe3O4/MWCNT hybrid nanofluid(1:4) shown the lowest. The results in this study indicated the thermal efficiency of evacuated tube solar collector was effectively enhanced by using Fe3O4/MWCNT hybrid nanofluids as working fluid comparing to the water and Fe3O4 nanofluid, the best performance of the evacuated tube solar collector was obtained when Fe3O4/MWCNT(1:4) hybrid nanofluid was used.

- **Keywords:** Nanofluid; Entropy generation; Entropy destruction; Exergy efficiency; Exergy destruction

S.C. Tiwari, A. Bhardwaj, K.D.P. Nigam, K.K. Pant, S. Upadhyayula. *A strategy of development and selection of absorbent for efficient CO2 capture: An overview of properties and performance*. Pages 244-273.

CO2 absorption using benign cost-effective absorbents is an essential unit operation not only in the process industry for CO2 separation and recovery from industrial off-gas streams but also for direct absorption from air to reduce the carbon footprint. Several absorbents are identified, by researchers, with high CO2 capture efficiency due to their favorable chemical and physical properties, interaction mechanism with CO2, and low regeneration energy cost. However, with the current Environmental Protection Agency (EPA) norms, more efficient low-cost benign absorbents need to be developed. Hence, the primary aim of this work is to comprehensively review various factors which are recently being considered in determining all these crucial parameters for best absorbents selection. The merits and demerits for establishing the physical and chemical absorbents have been discussed. Absorbent properties such as structural, transportation, and chemical properties are also discussed, along with various methods used to determine them. The pKa value based absorbent selection methodology seems an ideal way for absorbent selection. Further, the role of contactors for absorption performance is also reviewed, with a significant focus on the mass transfer coefficients, and the anal that a

circular microchannel reactor provides a 2–4 order of magnitude higher mass transfer coefficient value than a conventional reactor. The interaction mechanism of reactive absorbents has been discussed, as they show much better absorption kinetics. A comparative assessment of relative heat duties of these reported absorbents revealed that the catalyst doped, and blend amines systems provide lower regeneration heat duties. A relative cost of the absorption processes focusing on the recent ionic liquid solvent synthesis costs is described. Overall, this review provides a systematic insight that will assist researchers and engineers in understanding an absorption solvent's efficacy for CO2 capture comprehensively.

- **Keywords:** CO2 capture; Mass-transfer coefficient; Interaction mechanism; Regeneration heat duty; Cost estimation

Tomáš Prostějovský, Alena Kulišťáková, Martin Reli, Radim Žebrák, Kamila Kočí. *Photochemical treatment (UV/O3+UV/H2O2) of waste gas emissions containing organic pollutants in pilot plant unit*. Pages 274-282.

A continuous flow photochemical pilot plant unit containing a dry photolytic/photooxidation reactor UV185/UV254/O3 and an aqueous photochemical UV254/H2O2 reactor was used to remove VOC from the waste gas stream with a high flow rate. The efficiency of this system was thoroughly studied through the control of reaction conditions, the detection of intermediates, and the analysis of reaction products during the degradation of styrene, xylene, and their mixture. The conversion of the model substances depends on the initial concentration of the pollutant, the flow rate, and the type of pollutant. The highest conversion after passing through the whole pilot plant unit was achieved at an initial pollutant concentration 50 ppmv and a flow rate 100 m3·h−1, which is related to the residence time in the system. The conversion of styrene, xylene and their mixture after passing through the whole unit for the 100 m3·h−1 flow rate was 74%, 46% and 52%, respectively. Although the first dry photolytic/photooxidation reactor using UV185/UV254/O3 was more efficient for styrene degradation, the aqueous photochemical UV254/H2O2 part was more suitable for xylene degradation. These experimental results are in the agreement with carbon balance, which confirmed the outlet air contained only unconverted model pollutant (styrene, xylene or their mixture) and CO2. Figures of merit were calculated in order to evaluate the price efficiency of the technology. This study presents an effective AOPs system for the degradation of VOCs from waste gas streams with a high flow rate and provides an insight into their degradation pathways.

- **Keywords:** Advanced oxidation processes; Hydroxyl radical; Ozone; Hydrogen peroxide; Xylene; Styrene

Tania L. Gómez-Borraz, Armando González-Sánchez, Juan Cabello, Adalberto Noyola. Model assessment on the non-isothermal methane biofiltration at ambient conditions. Pages 283-297.

Direct anaerobic sewage treatment is increasingly adopted in several intertropical developing countries. The reduced carbon footprint of such facilities is based on its low electricity requirements and potential energy (biogas) recovery; however, if dissolved CH4 in the effluent is not controlled, this advantage will be drastically reduced. A suitable option to overcome this situation is to adopt CH4 desorption by an air stream, followed by bio-oxidation in compost biofilters. In such systems, the methanotrophic activity will increase the temperature in the biofilter to inhibiting values (above 40 °C), reducing the active volume of the compost media and its removal efficiency. This work addresses this process limitation, aiming to assess the temperature variations in the filter media and their effects on methane oxidation performance under different operating conditions. A

comprehensive mathematical 2-D porous-medium based model was developed and then calibrated and validated with experimental data. The model considers heat, momentum, and mass balances under non-steady-state conditions, including heat exchange at the biofilter container wall influenced by daily ambient temperature fluctuations and solar radiation. Results obtained from 6 model simulations at different operating conditions show that temperatures above 40 °C are reached at the center-upper zones of the compost biofilter due to the heat transported from the methanotrophic active zones located at the bottom (inlet) and container wall. At midday (12 – 14 h), solar radiation on the wall contributes 14% of the total heat gained in a non-covered biofilter. The model highlights the importance of facilitating heat transport from the compost media to the surroundings; some practical recommendations are presented for that purpose.

- **Keywords:** Compost biofilter; Effective porous medium; GHG; Metabolic heat; Outdoor conditions

Ran Gao, Chengzheng Tong, Hui You, Xiaorong Zhou, Xiaodong Huang, Mingzhang Pan. *Research on regeneration characteristics of diesel particulate filter based on fluid-thermal-solid coupling*. Pages 298-307.

In order to ensure that the diesel particulate filter (DPF) is not damaged during the regeneration process, a DPF regeneration model based on fluid-thermal-solid coupling is established. The temperature, stress and strain distribution during the regeneration process of DPF are analyzed, and the influence of stress and strain on the solid area of porous media under different carbon loads is revealed. The results show that there is an obvious local high temperature region in the center of the plug section of the intake channel and exhaust channel, and the tangential temperature of the inlet and exhaust outlet gradually decreases from the center to the surrounding. With the increase of carbon loads, the peak reaction temperature in the process of regeneration also began to rise. The thermal stress is mainly distributed near the side corners of the porous medium, and the maximum thermal stress is concentrated at the exhaust outlet end. The deformation is mainly concentrated in the solid center area of the plugs at both ends, the deformation amount decreases from the inside to the outside, and the deformation amount of the exhaust end is higher than that of the intake end. It can be found that the central area of the porous medium is the weak point of the structure, which is prone to thermal damage and cracks.

- **Keywords:** Diesel particulate filter; Active regeneration; Fluid-thermal-solid coupling; Stress distribution

Paulo Gabriel Siqueira, Márcio das Chagas Moura, Heitor Oliveira Duarte. *A Bayesian population variability based method for estimating frequency of maritime accidents*. Pages 308-320.

Industrial accidents, such as toxic spills, are one of the main causes of catastrophic environmental damage to animals and plants. The high number of vessels, including oil tankers that navigate the globe, increases the risk of potential oil spills affecting oceanic islands. The frequency estimation is a fundamental step in any risk assessment. However, this step presents shortcomings when dealing with rare, extreme accidents, i.e., low frequency/high consequence events. Classical statistical approaches are ineffective since available data are generally sparse and often censored in this context. To address this issue, we propose a Bayesian population variability-based method to estimate the distributions of accident rates. Based on that, it is possible to merge sparse data about accidents from various databases with the judgment of experts such as captains, pilots and chief officers. Finally, this method is applied to a real case of oil tankers that navigate nearby the Fernando de Noronha Archipelago, a UNESCO natural world heritage site in Brazil. The results can support risk assessments and provide

decision-makers with helpful information to better address measures to prevent accidents or reduce risks.

- **Keywords:** Bayesian variability analysis; Expert opinion; Maritime accidents; Frequency assessment; Quantitative risk assessment; Oil spills

Yuyuan Zhang, Kaili Xu, Ji Ge, Bo Liu. *Study on hydrogen evolution risk and suppression methods of Mg–Al/Mg–Zn alloy waste dust in wet dust collector*. Pages 321-329.

Mg alloy waste dust can react with water to produce hydrogen in the production of Mg alloy products, which has the possibility to lead to fires or explosions. Firstly, from the perspective of safety management, this paper systematically studies the impact of the difference of hydrogen evolution amount of magnesium based alloy waste dust particles(Mg–Al/Mg–Zn) on the risk of wet dust collector under different environmental conditions, and a two-stage hydrogen evolution model was constructed. Secondly, from a technical point of view, a method of using environmentally-friendly, cost-effective sodium phosphate to inhibit the hydrogen evolution reaction of Mg alloys is also proposed. The morphologies of Mg alloy dust particles before and after reaction were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), and chemical dynamics modeling before the related reaction mechanisms were identified. The research outcome of the present study could provide effective technical guidance for preventing hydrogen explosion accidents at Mg alloy fabrication facilities.

- **Keywords:** Mg–Al dust particles; Hydrogen production; Mg–Zn alloy dust particles; Alloy phase; Hydrogen explosion

Bing Wang. *Using an evidence-based safety approach to develop China's urban safety strategies for the improvement of urban safety: From an accident prevention perspective*. Pages 330-339.

Accidents (such as hazardous chemical accidents and fires) have adverse effects on urban safety and sustainable development. Many countries, such as China, are making great efforts to develop better urban safety strategies to prevent and mitigate accidents in urban areas and to keep cities safer. At national level, and from an accident prevention perspective, this study uses an evidence-based safety approach to propose potential strategies for China's urban safety. The contributions include: (1) the identification and discussion of major urban safety problems and challenges in China, and (2) the development of China's urban safety strategies based on available evidence. This study attempts to provide useful evidence and suggestions for future urban safety management, both within China and in other countries. However, because this paper discusses China's urban safety at macro level, more detailed studies on China's urban safety should be carried out for a deeper understanding and a more targeted solution for China's urban safety.

- **Keywords:** Urban safety; Urban sustainability; Evidence-based safety (EBS) approach; Accident; China

Linchao Ma, Jingkui Mao, Mohammad Marefati. *Assessment of a new coal-fired power plant integrated with solid oxide fuel cell and parabolic trough solar collector*. Pages 340-352.

Despite the major challenges facing fossil fuels, they are now utilized to supply nearly 80% of the world's energy requirements. Of this amount, about 30% relies on coal-based power plants. Such power plants emit large volumes of pollutant gases into the atmosphere, which has led to serious environmental crises. Therefore, the exploitation of

green technologies and/ or the integration of environmentally friendly systems in existing power plants are essential. The aim of the article is to introduce and conceptual-thermodynamic design of a lignite coal-based plant that is integrated with monoxide-hydrogen fueled solid oxide fuel cell (SOFC), and parabolic trough solar collector (PTSC) based-solar farms. The present paper provides energy, exergy, and thermodynamic analyzes with considering entropy generation and emission rate of the power plant. In addition, a comparison of system performance when using anthracite instead of lignite is also provided. Also, real climatic data (i.e., Yazd, Iran) have been used to evaluate the behavior of solar fields. The results showed that nearly 93.7 kg/s of gas is raised from the power plant after the combustion process. In addition, proposed power plant has energy and exergy efficiencies of 70.95% and 35.7%, respectively. Moreover, the PTSC2 solar farm in a lignite-fired power plant should have approximately 6.76-fold larger area than that of anthracite.

- **Keywords:** Coal gasification; Parabolic trough solar collector; Solid oxide fuel cell; Emissions; Energy and exergy

Xin Wang, Yiwei Zhong, Yuzheng Kang, Jintao Gao, Zhancheng Guo. *Promoted acid leaching of Zn from hazardous zinc-containing metallurgical dusts: Focusing on transformation of Zn phases in selective reduction roasting*. Pages 353-361.

As hazardous wastes from metallurgical processes, high zinc dust (HZD) was considered as a potential alternative resource of Zn. The acid leaching of HZD was a principal step and therefore was highly relevant to efficient utilization. Unfortunately, zinc ferrite ($ZnFe_2O_4$) in HZD was difficult to be leached by hydrometallurgical methods. Therefore, in this study, to enhance the recovery of zinc, selective reduction roasting was used to decompose $ZnFe_2O_4$. The transformation of Zn phases during the reduction process was investigated by thermodynamic calculation, XRD analysis. The results showed that $ZnFe_2O_4$ was converted into acid-soluble ZnO in H_2 at 600 °C, while the further reduction of ZnO to Zn(g) and the volatilization of ZnO was avoided. However, the soluble $ZnSO_4$ in HZD was also reduced to acid-insoluble ZnS. Consequently, a novel method of reduction roasting combined with water leaching was proposed to pretreat HZD. In water leaching, the solid-liquid ratio was1:10 (g/mL). When H_2SO_4 concentration was 80 g/L, the leaching ratio of Zn was 94.24% after pretreatment, higher than that of direct leaching of HZD (87.76%). Therefore, acid leaching of Zn was promoted by water leaching and reduction roasting pretreatment, which will bring considerable benefits to the high zinc dust recycling enterprises.

- **Keywords:** High zinc dust; Zinc ferrite; Reductive decomposition; Acid leaching; Phase transformation

Kun-Huang Chen, Ssu-Han Chen. *Applying an artificial intelligence model using multidimensional spatial-temporal data to predict arsenic contamination of groundwater*. Pages 362-367.

Special attention has been paid in recent years to the social and environmental implications of municipal solid waste. There are potential social and environmental issues associated with storing any waste in landfill. Soil, groundwater, and surface water contamination are issues related to landfill and the migration of contaminants by leaching to adjacent areas. The current research attempts to simulate the penetration of landfill contaminants through groundwater leaching, using PART modeling approaches. Multiple social factors, taken from five years of data from 20 counties and cities in Taiwan were used as predictors of groundwater arsenic content. The results indicate that the proposed model attains a precision rate of 87%. The findings suggest that county and city demographics and the volume of waste removed are two major factors in determining

the arsenic content of groundwater. The proposed predictive model can be adopted by agencies as an effective early warning tool for groundwater arsenic levels.

- **Keywords:** Groundwater; Arsenic; Artificial Intelligence; Multidimensional spatial-temporal; Water management; Sanitation and hygiene

G. Yu. Bivol, S.V. Golovastov, V.V. Golub. *Investigation of hydrogen-air and acetylene-air flame propagation through porous media using infrared visualisation*. Pages 368-383.

One of the modern energy safety concerns is ensuring explosion safety when working with flammable gases. For this purpose, various methods are used, such as active chemical inhibitors and passive combustion suppression. The use of various porous materials is prevalent among passive methods for combustion suppression. This study focused on the experimental investigation of hydrogen-air and acetylene-air flame propagation through polyurethane foam and through the empty channel. The use of high-speed infrared camera enabled visualization of flame propagation inside the porous material. Two types of diagnostic channels were used with the dimensions of the diagnostic section 16 × 20 mm and 40 × 20 mm. The length of the foam was 120 mm. In hydrogen-air mixtures with 10 pores per inch (PPI) polyurethane foam the flame velocity was higher than in the empty section; with 30 PPI polyurethane foam the flame was quenched in the mixture with equivalence ratio ER = 0.3, but for mixtures with ER = 0.4 and ER = 0.5 the average flame velocity was higher than in the empty channel. In the acetylene-air mixtures flame velocity was usually lower in polyurethane foam and only reached the flame velocity in the empty channel with ER = 0.8 and 10 PPI foam. Critical Peclet numbers that allowed the flame to propagate through porous materials were calculated based on the obtained experimental data. The critical Peclet numbers were 23–24 for the hydrogen-air mixture and 37–38 for the acetylene-air mixture. The channel was open near the ignition point, which allowed the obtained results to be less dependent on the channel length. Information obtained in this work can be used to improve the means of ensuring explosion safety, including in the areas of nuclear power and transport using hydrogen.

- **Keywords:** Hydrogen; Acetylene; Porous material; Flame quenching; Explosion safety; Infrared visualization

Linbo Qin, Jia Song, Wangsheng Chen, Guangqian Luo, Jun Han. *FeMn/Al2O3 as a high-efficient and low-cost catalyst for chlorobenzene removal in a nonthermal plasma-catalysis reactor*. Pages 384-394.

Fe and Mn are the transition-metals that have advantages of low cost and easy availability. In order to high-efficient remove chlorinated volatile organic compounds (CVOCs), a series of high-efficient and low-cost FexMny/Al2O3 catalysts were synthesized by reflux-coprecipitation method, and the removal of chlorobenzene, a CVOCs model compounds, was studied in a nonthermal plasma coupled with FexMny/Al2O3 system at room temperature. The kinetic parameters of the chlorobenzene removal in the nonthermal plasma reactor coupled with FexMny/Al2O3 were obtained. Meanwhile, the reaction route of the chlorobenzene removal in the nonthermal plasma coupled with FexMny/Al2O3 reactor was revealed. The results indicated that the best conversion efficiency and the highest CO2 selectivity of the chlorobenzene removal in the plasma-Fe1Mn1/Al2O3 system were in sequence as 95.77% and 93.11%. Moreover, the positive synergy between the plasma and the FexMny/Al2O3 catalysts greatly reduced the activation energies of the chlorobenzene removal, and improved the chlorobenzene removal efficiency in the plasma-FexMny/Al2O3 system. Finally, the possible reaction routes of the chlorobenzene removal in the plasma-Fe1Mn1/Al2O3 system were proposed based on the intermediates identified by the GC/MS.

- **Keywords:** Chlorobenzene; Plasma-catalysis; FexMny/Al2O3; Removal pathways

Dániel Krakkó, Bjørn Tobiassen Heieren, Ádám Illés, Kristin Kvamme, Sándor Dóbé, Gyula Záray. *(V)UV degradation of the antibiotic tetracycline: Kinetics, transformation products and pathway*. Pages 395-404.

Tetracycline (TETR) is an antibiotic drug that is widely used in both human and veterinary medicine. It is frequently detected in activated sludge, wastewater effluent, river and lake water or sediment, usually in the pg/L – μg/L concentration range, but sometimes above the mg/L level. Conventional wastewater treatment plants have low removal efficiency for a large number of small organic molecules including TETR. Their efficiency can be increased by applying e.g., an advanced oxidation method for the post-treatment of the wastewater effluent. One possibility is the use of (V)UV lamps for simultaneous disinfection and micropollutant removal. In this paper, the degradation of TETR by UV (λ = 254 nm) and (V)UV (λ = 185 nm and 254 nm) light was studied, focusing on kinetics, mineralization, transformation products and degradation pathways. The effect of dissolved oxygen during irradiation was also examined. As expected, the degradation rate of TETR drastically increased in (V)UV irradiation compared to the conventional UV light. The degradation rates increased by 9% and 16% in UV and (V)UV experiments in the presence of dissolved oxygen possibly due to the generation of additional oxidative radical species. Total organic carbon removal was generally 15%, high TOC removal could only be achieved with greatly increased photon flux in (V)UV photooxidation. In total, eleven aromatic transformation products (TPs) were identified during the irradiation experiments. Three TPs (TP 418, TP 398 and TP 383) were described for the first time. The main degradation pathways include loss of water, CO, methyl or dimethylamine groups. Based on the kinetic profiles, (V)UV irradiation could effectively degrade all aromatic transformation products.

- **Keywords:** Advanced oxidation processes; Pharmaceuticals; Persistent organic pollutants (POPs); Contaminants of emerging concern; UV-C; VUV/UV

Abhay Guleria, Rahul Singh, Sumedha Chakma, Volker Birke. *Ecological and human health risk assessment of chromite ore processing residue (COPR) dumpsites in Northern India: A multi–pathways based probabilistic risk approach*. Pages 405-420.

In this study, ecological and human health risk assessment (HHRA) of the subsurface environment was performed due to the presence of six different contaminants, i.e., Cr(VI), U, F-, As, NO3-, and Mo, in the proximity of chromite ore processing residue (COPR) dumping sites of Northern India. The analysis covered a probabilistic risk assessment approach comprised of 10,000 Monte Carlo simulations (MCS) for multi-exposure scenarios following soil and water pathways. The results of ecological risk indexes indicated considerable (contamination factor (CF) = 5.6) to very high (maximum CF ~ 11.0) contamination of soil near the Rania contaminant site. The maximum and 95th percentile of CF obtained due to Cr(VI) were 4.547 and 11.129, respectively, during the monsoon season. Cancer risk (CR) value for dermal contact exposure via soil pathway for the Rania site was > 1–2 orders higher than the safe limit, posing a serious threat to human health. Further, oral ingestion and skin dermal exposure to groundwater in the proximity of Chhiwali dumping site were posing the highest risk with CR = 18.5 and 54.9 (>10−6), respectively to the adult population. Overall, the study recommends an urgent need to take intensive remediation action for these COPR dumpsites to ensure human health safety.

- **Keywords:** COPR waste; Ecological risk index; Human health risk assessment; Soil adherence factor; Monte Carlo simulation

Özkan Köse, Yıldız Koç, Hüseyin Yağlı. *Is Kalina cycle or organic Rankine cycle for industrial waste heat recovery applications? A detailed performance, economic and environment based comprehensive analysis*. Pages 421-437.

Contrary to the increase in energy demand throughout the world, fossil fuels, which are the main energy source, is now more difficult to reach because of the pandemic, transport or bilateral relations, etc. These obstacles in obtaining fossil fuels reveal the need to minimize energy wastage by utilizing low-temperature waste heat sources releasing the atmosphere without use. Especially for the industrial fields usage of advanced heat recovery systems is necessary. In addition, it is a remarkable point that the evaluation of low-temperature thermal energy potential will contribute significantly to the reduction of carbon emissions, which is one of the most important goals in developed and developing countries. In this study, Kalina and Organic Rankine cycles, which are the most important low-temperature energy conversion systems in the utilization of low-temperature industrial waste heat with a temperature of 250 ºC and a mass flow of 10 m/s, were examined and compared to each other in terms of energy, exergy efficiency, economic outlook, and environmental effects. During the study, the turbine inlet pressure of the Kalina cycle was selected as 60, 90 and 120 bar, while the turbine inlet pressure of the organic Rankine cycle increased from 10 bar to the critical pressure of the fluid. For all selected pressure levels, the turbine inlet temperature was increased from the saturated vapor temperature of the fluid to 240 ºC. As a result, although the Kalina cycle was found economically better than the organic Rankine cycle (3.93 years), the organic Rankine cycle using n-Pentane showed a better performance than the Kalina cycle in terms of energy, exergy, and CO2 emission reduction. The thermal efficiency, exergy efficiency, payback period, and CO2 emission reduction value of the organic Rankine cycle with n-Pentane were calculated as 25.95%, 71.77%, 4.03 years, and 207.17 kg-CO2/h, respectively.

- **Keywords:** Industrial waste heat; Organic Rankine cycle (ORC); Kalina cycle (KC); Optimization; Environmental analysis; CO2 emission; Exergy

Shi Yong, Zhang Linzi. *Robust deep auto-encoding network for real-time anomaly detection at nuclear power plants*. Pages 438-452.

Detecting anomaly conditions in nuclear reactor is a critical issue in safety management of Nuclear Power Plants (NPPs). Conventionally, the operating status are monitored in transient data with pre-designed labels by human operators or basic diagnosis systems. Nowadays, continuous time series data from multi-sensors are increasingly collected and emerging unlabeled abnormal status are monitored during the operation, making it challenging to capture both spatial and temporal dependency at each time steps without supervised labels. In this paper, a robust unsupervised Multi-Variate Convolutional GRU Encoder-Dncoder (MVCGED) method is proposed to perform anomaly detection and fault diagnosis in multi-sensor operation time series data. Specifically, MVCGED first construct each time steps into signature matrices to maintain both spatial and temporal features via sliding windows with inner-correlation and forget mechanism. Subsequently, A CNN feature extraction network, CNN-based GRU encoding network and CNN decoding network are implemented successively to capture and reconstruct the hidden patterns of the signature matrices. Finally, the reconstruction loss are further utilized to detect anomalies and diagnose faults. Extensive empirical studies based on PCTRAN nuclear power plant operation data demonstrate that MVCGED outperforms commonly-used baseline methods.

- **Keywords:** Nuclear Power Plant; Anomaly detection; Multi-sensor; Time series; ConvGRU

Shuaishuai Li, Wei Zeng, Ziyue Jia, Ziyan Ren, Xiaojing Peng, Yongzhen Peng. *High-efficient phosphate removal from wastewater by weak magnetic La(OH)3 modified platanus biochar*. Pages 453-463.

An adsorbent of weak magnetic La(OH)3 modified platanus biochar (La-MB) was synthesized for phosphate (P) removal by iron lanthanum sequential modification method for the first time. Compared with synchronous modification method, La-MB had higher P adsorption capacity and similar magnetic separation property. The performance of La-MB was evaluated in terms of adsorption isotherms, adsorption kinetics, coexisting competitive substances, regenerative ability, and it as fixed-bed column filler to remove P from actual wastewater. The results showed that La-MB had a monolayer P adsorption capacity of 116 mg/g in the pH range of 3.0–9.0 at 35 ℃ with the contact time of 45 min, and the adsorption capacity was higher than most La-modified magnetic adsorbents. The coexisting SO2–4, NO-3 and Cl- had no effect, while the HCO-3, CO2–3 and humic acid interfered with the removal of P due to competition for active sites on the surface of La-MB. Moreover, approximately removal efficiency of 97% was remained after three adsorption-desorption cycles in 1.0 mol/L NaOH eluent, which showed the outstanding stability and cyclic utilization. The maximum treatment bed-volumes (BV) under influent flow rates of 0.5 mL/min, 1.0 mL/min and 1.5 mL/min were 3050 BV, 2000 BV and 1100 BV, respectively. The characterization results of zeta potential, FTIR and XPS revealed that the P adsorption of La-MB was dominated by ligand exchange, inner sphere complexation and electrostatic attraction. All results indicated that La-MB could serve as a promising adsorbent for the efficient removal of P from actual wastewater.

- **Keywords:** Phosphate removal; High-efficient adsorption; Weak magnetic; Biomass biochar; Sequential modification

N. Schmidt, J. Denecke, J. Schmidt, M. Davies, T. Heidermann. *Experimental investigation on condensation inside of storage tanks during rapid cooling in a heavy rain event*. Pages 464-474.

Experiments have been performed on a 2.6 m3 gas and liquid filled vertical storage tank at ambient conditions that has been cooled with cold water. The breathing volume flow and main parameters, such as gas and wall temperatures, condensate masses generated and tank differential pressure have been measured. The experiments have been performed with dry air, water and methanol as storage media. The aim is to obtain validation data for future models and correlations for cooling of storage tanks. Additionally, the impact of fog formation in the tank atmosphere, dropwise and film condensation and rain intensity during heavy rain events on the maximum breathing flow rate have been investigated. As a result of the analysis of physical phenomena during the cooling of the tank, an increase in the maximum breathing volume flow for storage media with increasing vapor pressure was observed. Strong fog formation was visible in all experiments with condensable liquids. In contrast to alcoholic storage media, dropwise condensation on the wall is expected when storing aqueous media. Rain intensity and heat transfer models from literature were examined regarding the sizing of tank breathing valves. Deviations between experimental data and a typical manual calculation model for sizing of tank breathing devices varied between 13% and 143%. The validation on the experimental data clearly showed that current models are not suitable for describing the breathing volume flow rate that occurs during sudden heavy rain events with sufficient accuracy.

- **Keywords:** Loss prevention; Vacuum damage; Heat transfer; Storage tank; Condensation

Ana A. Márquez, Oscar Coreño, José L. Nava. *An innovative process combining electrocoagulation and photoelectro-Fenton-like methods during the abatement of Acid Blue 113 dye*. Pages 475-486.

This paper focuses on the implementation of a smart hybrid water treatment process that combines electrocoagulation (EC) and active chlorine-based photoelectro-Fenton-like (PEF-like) methods to remove Acid Blue 113 (AB 113) dye, used as a model persistent organic pollutant (POP), from synthetic solutions containing chlorides. The composition of AB 113 solutions expressed in terms of chemical oxygen demand (COD) was 250–1000 mg L-1 in 2000 mg L-1 NaCl at neutral pH. EC is conceived as a dye removal process, where iron flocs partially remove the dye in high concentrations. The residual dye in the solution (after EC) is oxidized to CO2 in the PEF-like treatment. An up-flow EC reactor was used for EC with two Fe plates as anode and cathode. A filter-press cell with a Ti|Ir-Sn-Sb-oxides anode and a stainless-steel cathode was employed for the PEF-like process. During PEF-like, the chloride is oxidized to HClO, reacting with residual Fe2+ from the EC to yield •OH. In EC, the influence of the electrolyte flow velocity ($0.69 \leq u \leq 3.47$ cm s−1), applied current density ($6 \leq j \leq 18$ mA cm−2), and initial AB 113 dye on the COD and color removal were systematically examined. The solution after EC was handled by PEF-like at u = 24.2 cm s-1, j = 15 mA cm-2, adjusting 0.4 mM Fe2+. The best conditions of EC were j = 18 mA cm-2 and u = 0.69 cm s-1, reaching COD removals from 67%. After EC, the residual COD was treated by PEF-like, reaching the complete abatement of organic matter. The total operating costs of the treatment (EC + PEF-like) ranged between 1.36 and 1.39 USD m-3. SEM-EDS, XRD, FTIR, and organic elemental analysis (OEA) of the dry flocs confirmed the adsorption of AB 113 on iron aggregates. HPLC analysis during the PEF-like process allowed to identify traces of carboxylic acids at the end of the treatment.

- **Keywords:** Hybrid process; Electrocoagulation; Photoelectro-Fenton-like; Persistent organic pollutants; Iron flocs, Water treatment

Duanwu Yang, Jinyong Wang, Xiaoan Yan, Hongbin Liu. *Subway air quality modeling using improved deep learning Framework*. Pages 487-497.

Soft-sensing modeling of indoor air quality in subways is critical for public health. For the purpose of reducing monitoring costs and building health risk assessment models, a new deep learning forecasting model based on empirical mode decomposition, long short-term memory (LSTM) block and squeeze and excitation networks (SENet) is proposed. To begin, the original PM2.5 data is decomposed into multiple sub-series with varying frequencies using empirical mode decomposition. Then, an LSTM neural network is built to forecast the new sub-series. Finally, squeeze and excitation networks were constructed and coupled to automatically pick informative weights to obtain the real-time forecasting result. The proposed model is compared to other commonly used models such as convolutional neural network and LSTM for its ability to forecast PM2.5 on an hourly experiment. The proposed model outperforms reference models in terms of forecasting performance, owing to its ability to capture informative characteristics and temporal patterns from varying PM2.5 dataset. The mean square error is improved by 38.29% and 29.21% compared with convolutional neural network and LSTM, respectively. When compared to convolutional neural networks and LSTM, the mean absolute error is reduced by 22.93% and 13.38%, respectively. Moreover, the proposed model also performs best in health risk warning assessment.

- **Keywords:** Indoor air quality; Empirical mode decomposition; Long short-term memory; Squeeze and excitation networks; Soft sensor; Health risk warning assessment

Rui Qi. *Novel thin-film nanocomposite membranes with crosslinked polyvinyl alcohol interlayer for Perfluorinated Compounds (PFCs) removal*. Pages 498-505.

Conventional polyamide-based interface polymerized nanofiltration (NF) membranes exhibit trade-off characteristics between water permeability and salt selectivity. The introduction of nanomaterial interlayers into thin-film composite (TFC) membranes is expected to overcome the limitation. Herein, a novel membrane was constructed via coating a polyvinyl alcohol (PVA) interlayer on the PES supporting film. Trace amounts of MXene nanosheets were used to form a barrier to avoid the occupancy of large pores by PVA. Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), Raman spectra, water contact angle (WCA), zeta potential, and other characterizations were used to evaluate the chemical and physical properties of the prepared membranes. Due to the PVA hydrophilicity, the composite membranes achieved higher hydrophilicity. Besides, the electronegativity enhancement and roughness improvement facilitate the film to have better application prospects. At the lab scale, the optimized membranes achieved a high-water flux of 22.8 L $m^{-}2h^{-}1bar^{-}1$ and a 94.5% MgSO4 rejection. The typical kinds of PFCs, including PFOA, PFOS, PFHxA and PFBA, were quantitatively evaluated and analyzed by electrostatic interaction. The excellent performance was maintained in the case of environmental changes owing to the stableness of the PVA interlayer. This study provides a new avenue for fabricating robust NF membranes for actual production.

- **Keywords:** Nanofiltration; TFNi membranes; Polyvinyl alcohol; Polyamide; MXene

Haibo Gao, Yuqiu Zhang, Yongqi Liu, Yanxia Wang, Peng Sun, Yuxiang Ma, Zehong Gu, Wenbo Yu. *Numerical simulation of heat transfer performance of different heat exchange tubes in heat recovery steam generator*. Pages 506-512.

For the purpose of reducing the cost of hydrogen production in process engineering and practice and enhancing the heat exchange efficiency of heat recovery steam generator, a new spring-blade mixed heat exchange tube was creatively put forward, and the performance evaluation criterion (PEC) was used as evaluation index of comprehensive heat transfer performance. To explore the heat transfer performance, the velocity distribution, temperature distribution, pressure distribution and comprehensive heat transfer performance were analyzed, and heat transfer coefficient and the value of PEC were obtained. The addition of spring and blade in the mixed heat exchange tube has obvious positive impacts on the velocity, temperature and pressure drop. In the Reynolds number range of 20000–40000, the heat exchange coefficient increment of the mixed heat exchange tube is increased by 35% and 45% than that of the spring and blade heat exchange tube respectively. The pressure drop is positively correlated with the heat exchange coefficient, and its increase leads to the decrease of PEC value.

- **Keywords:** Heat transfer performance; Mixed heat exchange tube; Spring; Blade; Hydrogen production

Hiba R. Mohammed, Saba A. Gheni, Khaleel I. Hamad, Safaa M.R. Ahmed, Omar A. Habeeb, Marwan A. Mahmood. *Synthesis, evaluation, and optimal stability of a biowaste-based catalytic oxidative desulfurization of model fuel in a trickle bed reactor*. Pages 513-527.

Oxidative Desulfurization (ODS) is one of the promising alternative processes. However, the lifetime of the ODS catalysts is an issue that restricted the use of the process. In this work, Activated Carbon (AC) prepared from biowaste (apricot stones (AS)) was impregnated with Mn and coated with aluminum oxide to prolong the lifetime of the ODS

process. To evaluate the performance of the prepared catalysts for a continuous three-phase ODS process, a trickle bed reactor (TBR) was used to conduct the ODS process at mild oxidation temperatures. The ODS evaluation study was conducted under different temperatures (60 and 70 °C), LHSVs (1, 1.35, 2, and 4 h-1), pressures (6 and 800 kPa), and initial sulfur concentrations (100 and 300 ppm). Both coated and uncoated catalysts showed high removal efficiency of the n-butyl mercaptan in the TBR. The maximum conversions obtained were 97.29 % and 95.19 % for the coated and uncoated Mn/AC catalysts at T = 70 °C, P = 800 kPa, LHSV= 1 hr-1, and initial sulfur concentration= 300 ppm. Besides the high performance, the coated Mn/AC showed outstanding stability during the continuous oxidation process. A kinetic model was formulated for the ODS process for the estimation of kinetic parameters of the high stability process. gPROMS has been used for modeling, simulation, and parameter estimation via optimization. The simulation results showed good consistency with the experimental data of all lumps with an absolute average error of up to 5 % and the optimization resulted in the optimal kinetics parameters of the high stability ODS process

- **Keywords:** Oxidative desulfurization; Biobased activated carbon; Coating; Stability; Naphtha

Guoxi He, Qing Zou, Kexi Liao, Jihui Leng, Shuai Zhao. Corrosion mechanism of high temperature and O2 content in steamed CO2/O2/SO2 system and failure behavior of 20G steel on steam-injection pipelines. Pages 528-542.

The corrosion mechanism and failure behavior of 20 G steel in steamed CO2/O2/SO2 environment (7.8 MPa, 100–301 °C) are studied. The surface characterization technology is adopted to analyze the corrosion rate and the microscopic morphology of corrosion product film, where the corrosive influencing factors are determined. The influence of temperature on the film formation kinetics is greater than that of cathodic reaction thermodynamics, wherein the corrosion product film has good performance for anti-corrosion. The interaction between H+ and Cl- leads to the degradation of mechanical properties. The residual-life evaluation model is proposed to recommend the reinspection period of the steam injection pipeline.

- **Keywords:** Steam injection pipeline; Corrosive CO2/O2/SO2; Temperature; Corrosion mechanism; Failure

Chaoying Li, Jie Hou, Wuyi Cheng, Wenmei Gai. *A multiagent-based modeling approach for emergency evacuation plan optimization during toxic gas releases within chemical plants*. Pages 543-557.

It is essential to minimize the gas exposure risk during evacuation in the event of toxic gas releases. This study uses a multiagent-based model to simulate the evacuation processes of a chemical plant and surrounding residential areas. An evaluation and optimization method for evacuation plans was proposed. A risk assessment model for ambient evacuation was established, and the evacuation plan optimization process was proposed. Using a chemical plant in Tianjin, China, as an example, the evacuation scenario of workers and surrounding residents after liquid ammonia release was simulated, and the effectiveness of the optimization strategies for the original evacuation plan is verified. The results reveal that using optimization strategies dramatically reduces the gas exposure risk during evacuation. The gas exposure risk during evacuation of some evacuation sub-areas is reduced by optimizing the evacuation route. Meanwhile, issuing the evacuation order sooner and optimizing the warning diffusion model exerts an excellent risk reduction effect on areas with low ammonia concentrations. Evacuation optimization strategies suitable for different evacuation sub-areas are not the same. They need to be determined according to the real situations of the evacuation sub-areas. The

results can help facilitate decision-making for the formulation and optimization of emergency plans for toxic gas releases.

- **Keywords:** Toxic gas releases; Emergency evacuation; Evaluation of evacuation exposure risk; Evacuation plan optimization; Multiagent-based modeling

Nabila Shehata, Khaled Obaideen, Enas Taha Sayed, Mohammad Ali Abdelkareem, Mohamed S. Mahmoud, AbdeL-Hay R. El-Salamony, Hamada M. Mahmoud, A.G. Olabi. *Role of refuse-derived fuel in circular economy and sustainable development goals*. Pages 558-573.

Refused derived fuel (RDF) is one of the products of the MSWs that is effectively used as an energy source, especially in the cement industry. This work discusses the role of the RDF in the achievement of the United Nations Sustainable Development Goals (SDGs) and the circular economy. Moreover, the barriers that challenge the widespread of the RDF are indicated. The RDF positively contributes to the most SDGs. However, the main contribution would be in SDG l: no poverty, SDG 3: good health and well-being, SDG 6: SDG 6: clean water and sanitation, SDG 7: affordable and clean Energy, SDG 8 decent work and economic growth, SDG 9: industry, innovation and infrastructure, SDG 11: sustainable cities and communities, SDG 12: responsible consumption and production, SDG 14: life below water and SDG 15: life on land. While in the main contribution of the circular economy comes from its ability to reuse municipal solid wastes, industrial solid waste, non-recyclable plastics, waste tires, biomass, paper/card, waste oils, and waste textiles. In addition, RDF will reduce the CO2 by up to 2155.3 106 Kt CO2/year and recover heat content from 2 to 5.5 Gcal/t. Moreover, the RDF will save up to 15% of the fuel that equals 4.92 tons/h. Such fuel reduction will save 486 USD/h in petcoke costs, with 2.27 tons/h of CO2 being emitted into the atmosphere at a net saving of 389 USD/h. The results guide academic researchers, policymakers, and stakeholders worldwide to evaluate solid wastes as alternative fuels concerning their overall sustainability and cheapness. Moreover, this work introduces some future research directions to involve solid wastes in circular economy and SDGs. Furthermore, a set of indicators are proposed to guide the stakeholder to increase the RDF contribution to SDGs and lower the possible trade-off.

- **Keywords:** Refused derived fuel (RDF); Municipal solid waste (MSW); Circular economy; Sustainable development goals (SDGs); Cement industry; Barriers

Shengyu Jiang, Guoming Chen, Yuan Zhu, Kang Liu, Yuanjiang Chang, Zhaoyang Wang. *Probabilistic approach for risk assessment of offshore hydrate wellbore during test production*. Pages 574-584.

The problem of wellbore risk due to complicated phase variation in coupled seepage in the process of hydrate production is one of a major obstacle restricting its commercial production. In response to this problem, a hybrid methodology for evaluating the risk of offshore hydrate test production wellbore is proposed using self-developed Particle Filter (PF) model, which realizes risk update through measurement data based on physical model. In this study, the physical model is constructed by a multi-field coupling model and the corresponding algorithm. The monitoring data is generated by Monte Carlo simulation to illustrate the method application. Then the probability prediction curve of the shear failure of the sediment around the wellbore can be calculated based on the PF. Finally, a novel dynamic risk matrix is developed to evaluate the risk of the current hydrate wellbore. A case study using geological parameters of hydrate sediments in the Shenhu area of the South China Sea was presented to illustrate the application of the proposed framework. Results indicated that the remaining safe production time at 90 days is between 210 days and 280 days, with a pressure drop of 3.0 MPa and 0.75 as the threshold. Subsequently, a dynamic risk matrix diagram of the risk of the hydrate

wellbore is proposed based on Event Sequence Diagram (ESD) and Bayesian Network (BN). The result shows that the risk of abandonment caused by landslides should be prevented in the early stage, and the workover risk caused by damage to the wellbore structure should be paid special attention to in the middle and late stages. The proposed methodology can provide applied technology for wellbore risk management in the process of hydrate test production.

- **Keywords:** Natural gas hydrate; Wellbore risk assessment; Partial Filter; Bayesian network

Ekta Singh, Rahul Mishra, Aman Kumar, Sushil Kumar Shukla, Shang-Lien Lo, Sunil Kumar. *Circular economy-based environmental management using biochar: Driving towards sustainability*. Pages 585-600.

There is a growing interest in developing "circular economy" with the major goal of eliminating waste by appropriate planning. Biochar has recently gained popularity in the environmental sector as a versatile material for waste reduction and increasing the efficacy of the circular economy. It has demonstrated possibilities towards environmental impact, battling climate change, and creating an efficient circular economy model. Despite these positive prognoses, research on biochar's benefits is still widely ongoing. This is interrelated to the biochar's inherent properties that are deeply impacted by certain variables like feedstock types and treatment conditions. In this review, the conversion of waste into biochar and its application in different regions have been discussed while considering the CE. It discusses how waste materials are upcycled to make biochar and then used towards betterment of the environment. It highlights how biochar can be produced from different wastes and can be used in agriculture, wastewater treatment, anaerobic digestion and various other sectors thereby proving its multidimensional role towards protection of the environment and successfully building up a circular economy based environmental management model. This finally ends up closing the loop thereby demonstrating an actual circular economy.

- **Keywords:** Circular economy; Biochar; Pyrolysis; Wastewater treatment; Environmental management

Gang Zhou, Bin Jing, Zhuo Xu, Bingyou Jiang, Rui Xu, Bo Ren, Biao Sun. *Simulation study on gas-bearing dust and its application combined with air curtain in development heading, a case study*. Pages 601-612.

In view of the problems caused by the overrun of gas and dust in the tunneling process of 7703 rock roadway in Zouzhuang Coal Mine, the risk control technology research was carried out by combining numerical analysis, research and development of new automatic wall-attached duct and field test, and the dust closed control within low gas concentration was realized. The results show that the gas concentration in the local area exceeded the legal or regulation limit of 1% under the conditions of forced ventilation, axial-to-radial flow ratio 1:9 and 2:8 mixed ventilation. When the axial-to-radial flow ratios were 3:7 and 4:6, the gas concentration was low, approximately 0.5%. Additionally, when the axial-to-radial flow ratio was 4:6, the dust concentration was still maintained at approximately 150 mg/m3 until 20 m away from the head. When the axial-to-radial flow ratio was 3:7, the dust pollution was effectively controlled. At approximately 17 m from the head, the average dust concentration was gradually brought lower than 4 mg/m3.

- **Keywords:** Whole rock fully mechanized driving face; Dust-laden gas mixture; Gas concentration; Air curtain dust control; Numerical calculations

Yi-Ju Wu, Hsin-Yu Chen, Ben-Chiau Chang, Fang-Shian Shiu, Kao-Sheng Lin, Ke-Fan Lin, Wan-Ru Chen, Tsair-Fuh Lin, Liang-Ming Whang. *Biological treatment of high strength monoethanolamine (MEA)-containing wastewater from printed circuit board manufacturing industry*. Pages 613-620.

Develop-etch-strip (DES) process in printed circuit board (PCB) manufacturing industries produces wastewater containing high organic nitrogen, in which monoethanolamine (MEA) is the main COD and nitrogen source. This study evaluated feasibility of biological treatment of high concentration MEA-containing acidified DES wastewater collected from a full-scale PCB industry. Batch test results indicated that aerobic conditions attained the highest specific COD degradation rates (6.5–14.6 mgCOD/gVSS/h), anoxic conditions attained second (4.81 mgCOD/gVSS/h), and anaerobic conditions was the lowest (1.3–3 mgCOD/gVSS/h). The anoxic/oxic (A/O) sequencing batch reactor (SBR) with porous polyurethanes carriers, BioNET, was able to treat MEA-containing acidified DES wastewater with 80 % COD removal and 23 % TN removal at influent COD of 300 mg/L, while the A/O continuous stirred tank reactor (CSTR) with BioNET at 8 h of HRT achieved above 96 % COD removal and 78 % TN removal at influent COD of 630 mg/L. The aerobic batch test results indicated that specific COD degradation rates followed a Haldane-type model, suggesting that MEA acts as an inhibitory substrate, especially at concentrations above 2000 mg/L. In addition, MEA inhibited the onset of nitrification, but not specific nitrate production rate, suggesting that MEA may inhibit nitrification by inhibiting expression of amoA gene, based on amoA gene expression results. Finally, the contribution for COD degradation, denitrification and nitrification by BioNET (< 20 %) was lower than that for suspended sludge in the A/O CSTR, suggesting that the role of BioNET carriers could retain microorganisms and served as the habitats for microorganisms to avoid washout at a shorten HRT situation.

- **Keywords:** Monoethanolamine (MEA); Develop-etch-strip (DES) wastewater; BioNET; Nitrification inhibition; amoA gene expression

Aboozar Gholami, Seyed Ali Jazayeri, Qadir Esmaili. *A detail performance and CO2 emission analysis of a very large crude carrier propulsion system with the main engine running on dual fuel mode using hydrogen/diesel versus natural gas/diesel and conventional diesel engines*. Pages 621-635.

Due to the fact that the emissions is a very important and challenging issue in our world today, especially for the shipping industry, so the use of more environmental friendly fuels in marine engines has become very attractive among researchers. The most interesting and promising alternative fuel is hydrogen (H2) and extensive research on feasible production and developing advance reliable consumption methods is ongoing. In this paper, the implication of hydrogen and performance of the propulsion system of a very large crude carrier is studied, by considering the speed required for the relevant marine voyage cycle to investigate and assessed when fuel is partially switched from diesel to hydrogen. Through developing an advance code in the Matlab-Simulink software, the effect of hydrogen percentage from 1 % to 10 % on CO2 emission and propulsion performance is assessed for the proposed marine voyage and the results are compared with the case of natural gas/diesel or solely conventional diesel. The modeling prediction indicates that by changing the composition of fuels used, at the same time trying to maintain the same power output and proper performance of the engine and propulsion system, the amount of CO2 emission could significantly be reduced, up to 10 % or even more than 24 % in the cases that the energy share of hydrogen and natural gas is 10 % and 99 % for dual fuel hydrogen/diesel and dual fuel natural gas/diesel engines, respectively.

- **Keywords:** Dual fuel engine; Natural gas; Diesel; Hydrogen; CO2; Very large crude carrier

Yicui Wei, Mengfan Wang, Wei Qi, Zhimin He. *Flame-resistant bifunctional MOF-based sponges for effective separation of oil/water mixtures and enzyme-like degradation of organic pollutants*. Pages 636-644.

Water pollutions that come from spilled oils, discharged organic reagents and abused pesticides have become an urgent problem to ecosystem. In this study, inspired by the multi-properties of MOF materials, we presented a bifunctional MOF-based sponge (OPA-UiO-66 @MF) to achieve the effective oil/water separation as well as the catalytic degradation of organic pollutants. On one hand, upon the in-situ growth of UiO-66 on melamine foam (MF) sponges and the octadecyl-phosphonic acid (OPA) modification of UiO-66, we highlighted the superhydrophobic/superoleophilic property of the OPA-UiO-66 @MF, which leads to excellent performances in oils adsorption and continuous oil/water separation. On the other hand, benefits from the lipase-like property of UiO-66, OPA-UiO-66 @MF was proved having potential ability in the catalytic degradation of carboxylic acid ester pesticides which are usually enriched in oils or organic solvents. Moreover, since phosphorus containing groups can be introduced onto the surface of sponge through OPA modification, OPA-UiO-66 @MF also displayed superior flame resistance. As an effective, safe and green material, the developed flame-resistant bifunctional OPA-UiO-66 @MF sponge might provide a promising application in the elimination of organic pollutants in water systems.

- **Keywords:** Melamine foam sponge; Metal organic frameworks; Oil/water separation; Catalytic degradation; Flame resistance

Hamad Gohar, Asif Hussain Khoja, Abeera Ayaz Ansari, Salman Raza Naqvi, Rabia Liaquat, Muhammad Hassan, Khalil Hasni, Umair Yaqub Qazi, Imtiaz Ali. *Investigating the characterisation, kinetic mechanism, and thermodynamic behaviour of coal-biomass blends in co-pyrolysis process*. Pages 645-658.

The integration of biomass into existing thermochemical conversion processes for bioenergy production is expected to play a key role in the energy transition to reduce the reliance on depleting fossil fuels and mitigate fossil carbon emissions. In this study coal-biomass blends containing hemp and sawdust were prepared with various blending ratios for co-pyrolysis. The coal-biomass blends were characterised using ultimate analysis (CHN), gross calorific value (GCV), FTIR, and TGA. Co-pyrolysis was performed in TGA that was applied to study the thermokinetic behaviour of the respective blends. The deviation between the experimental and calculated values of TGA mass loss (ML), the residue left (RL), and maximum mass loss rate (DTGmax) were calculated to observe the synergistic effect. The positive deviation in the ML and DTGmax values indicated the presence of a synergistic effect during co-pyrolysis. Kinetic parameters were analysed by employing the Coats-Redfern method with thirteen integral functions. The activation energy (Ea) for individual coal was 39 kJ/mol through a one and a half chemical reaction (F3/2), while individual sawdust and hemp showed 60 kJ/mol through a deceleratory reaction mechanism for contracting sphere (R3) and 44 kJ/mol through the second-order chemical reaction (F2), respectively. Thermodynamic parameters such as the change in enthalpy (ΔH) and change in Gibbs free energy (ΔG) showed positive values that indicate the reaction was non-spontaneous. Additionally, the change in entropy (ΔS) was negative that suggested a more ordered state. The coal-sawdust blends were found to be suitable for the production of bio-oil as the individual sawdust contained a higher number of volatiles, whereas the coal-hemp blends were better suited for the production of biochar since the individual hemp produced more residue after co-pyrolysis. Hemp biochar was

further characterised by FTIR, TGA, GCV, and SEM-EDX analysis to investigate its potential in environmental and energy applications.

- **Keywords:** Hemp pyrolysis; Coal-biomass blends; Co-pyrolysis; Synergistic effects; Kinetics & thermodynamics; Biochar

Chuchai Sronsri, Napong Panitantum, Wanpasuk Sittipol, Kongpop U-yen, Pongsathorn Kerdphol. *Optimization of selective gold recovery from electronic wastes through hydrometallurgy and adsorption*. Pages 659-668.

The feasibility of hydrometallurgy for metal extraction from electronic wastes was investigated in the current work. Samples were ground and preliminary extracted by nitric acid and aqua regia. The gold concentrations in nitric acid and aqua regia were measured as 1.82 mg L1 and 29.45 mg L1, respectively. In addition, extraction performances using Cl2 (oxidizer) were studied. Experiments were conducted by connecting an extraction reactor to an oxidizing electro-generator. It was found that copper and gold were mostly extracted by adjusting different extraction conditions, such as extraction time, HCl concentration, extraction temperature, current density, particle size range, sample mass (solution density), and stirring speed. Two specific extraction steps were employed to selectively extract copper and gold. It was detected that 98.1 % of copper was extracted using the first extraction step twice, whereas, in the final step, 95.1 % of gold was extracted from the residue sample of the first step. The gold recovery performances of five different resins were investigated, and IRA402 Cl and HPR9700 resins manifested the highest adsorption ability and selectivity. The adsorption mechanism was found to be a monolayer adsorption process, and the adsorption capacities of IRA402 Cl and HPR9700 resins reached 303.8 mg g1 and 295.4 mg g1, respectively. Finally, gold desorption from these resins was successfully performed using an acetone-HCl mixture as the eluent. Reusability tests revealed that these two resins could be reused at least 6–7 times with an adsorption capacity loss of less than 10 %.

- **Keywords:** Electronic waste; Hydrometallurgy; Oxidizer; Selective extraction; Gold recovery; Resin

Mohammad Hossein Keshavarz, Zeinab Shirazi, Paria Eskandari. *A simple assessment of toxicity towards Chlorella vulgaris of organic aromatic compounds in environmental protection*. Pages 669-678.

A new approach is introduced for the assessment of toxicity to living organisms from the deposition of different types of organic aromatic compounds in the aquatic environment. Several simple models are introduced for reliable prediction of pIC50, pIC20, pLOEC, and pNOEC towards Chlorella vulgaris (C. vulgaris) of organic aromatic compounds. They need structural parameters as simple descriptors rather than complex descriptors, which are used in the available quantitative structure-activity/toxicity relationship (QSAR/QSTR) models. The largest available reported data of pIC50 for 145 aromatics are used to obtain suitable simple descriptors. A core correlation is introduced for estimating pIC50, which is based on the number of chlorine atoms and molecular weight as well as the contributions of nitro groups and intramolecular hydrogen bonding in phenol derivatives under certain conditions. Its reliability is improved by considering two isomeric structural parameters. Reliable models for pIC20, pLOEC, and pNOEC are also derived and tested using six descriptors. Since the outputs of available QSAR/QSTR models are restricted to phenol and aniline derivatives, the predicted results of the new models are compared with the reported data of one of the best available complex QSAR/QSTR models. Various statistical parameters confirm that the models for pIC50, pIC20, pLOEC and pNOEC show high reliability as well as accuracy, precision, and suitable goodness-of-fit. For example, the predicted results of root mean squared error

(RMSE) of pIC50 for 67 and 13 of training-test and external chemical sets of the new/QSTR models are 0.256/0.285 and 0.215/0.376, respectively.

- **Keywords:** Toxicity; Chlorella vulgaris; Molecular structure; Organic aromatic compound; QSAR/QSTR

Zeinab Masalegooyan, Farzad Piadeh, Kourosh Behzadian. *A comprehensive framework for risk probability assessment of landfill fire incidents using fuzzy fault tree analysis*. Pages 679-693.

Landfill fire is the most frequent type of incident in the waste management complexes. This paper presents a new framework for risk probability evaluation of major fires in landfills using the fuzzy fault tree analysis. The framework starts with construction of the fault tree of landfill fire comprised of 38 basic and 22 intermediate events with the corresponding type of faults under managerial, executive, human, and environmental conditions. Fault tree quantitative analysis is carried out through a combination of fuzzy set theory and experts' judgements to overcome the lack of data. Two new sensitivity analysis approaches are used to identify the critical fault type and critical paths in the fault tree. The proposed framework is demonstrated by its application to a real-world case of a landfill in Iran. The results show the probability of a major "fire incident" is 5.5 %, whereas "fire occurrence" stands for 25 % probability, higher than "lack of preparation for controlling fire" with 21.60 % probability. In addition, "Waste's uncontrolled dumping" is recognised as the highest critical event with a failure probability of 6 % and importance degree of 24 %. "Executive fault" is also found as the most fault's critical type through sensitivity analysis. The results also reveal the major impact of the experts' weights, especially for events related to human or management faults. These results can give decision-makers a profound insight into providing effective intervention strategies for minimising the risk of major landfill fire incidents.

- **Keywords:** Comprehensive evaluation; Fuzzy fault tree analysis; Landfill fire incidents; Probability assessment; Sensitivity analysis

Ahmad Fahmi, Raman Ahmadi, Mohammad Yousef Memar, Salar Hemmati, Samira Babakhani, Hossein Samadi-Kafil, Hooshang Katebi, Samira Haghighatara. *A novel microbial-assisted method for sodium bicarbonate production – Cleaner production, safe and facile synthesis*. Pages 694-702.

The human tendency to new, cleaner, and safer methods for the production of materials has led to extensive eco-friendly studies. Herein, urea ((NH2)2CO) was exposed to bio-catalyzed urease enzyme from Sporosarcina pasteurii (formerly known as Bacillus pasturii). After hydrolysis of urea, the gassing of CO2 led to the production of sodium bicarbonate (NaHCO3). The final product was validated for its crystallographic, microstructural, and elemental properties through X-ray diffraction (XRD), carbon-hydrogen-nitrogen (CHN) elemental analysis, field-emission scanning electron microscopy (FE-SEM), X-ray fluorescence (XRF) spectroscopy, and energy-dispersive X-ray (EDX) spectroscopy. These results, along with the chemical evaluation of chloride ion, proved that NaHCO3 was the major compound with a purity of > 76 %. This finding confirmed that cleaner and facile production of NaHCO3 is possible by our defined novel enzymatically-modified Solvay method. Besides removing hazardous materials before and after the process (raw materials and residues), this method simultaneously highlights the potential for converting CO2 captured from the environment or gases released from different industries to NaHCO3 a highly applicable material for pharmaceuticals, food, and other industries.

- **Keywords:** Bioprocessing; Cleaner production; Sporosarcina pasteurii (Bacillus pasturii); Sodium bicarbonate (NaHCO3); Urea hydrolysis; Environmental pollution

Venkatasubramanian Sivakumar. *Towards environmental protection and process safety in leather processing – A comprehensive analysis and review*. Pages 703-726.

Leather process industry requires in-plant process interventions with inherent safety; wherein, enhancement in process efficiency, rather than end-of-pipe treatment are gaining importance. Switching over to alternate processes with statutory requisite such as material safety and toxicological information of chemicals employed, eco-label, Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) and UN's Sustainable Development Goals (SDGs) for Leather sector (SDGs) are essential. Herein, these aspects have been linked with safer and eco-benign process development. The present review analyze the environmental, occupational safety concerns and difficulty in overcoming the conventional non eco-benign chemicals, in order to develop alternative cleaner processes through scientific basis with fundamental theory and practice of leather manufacture. Aspects such as mass balance, diffusion phenomena, E-Factor metrics for assessing the clean technology and pollution reduction have been explained. Focus given towards improving exhaustion levels in various stages, eco-benign processes, non-toxic products, use of natural materials, bio-process, novel processes/products, new process systems, 3 R approach, process intensification tools such as ultrasound are analyzed with environmental and cost aspect. In addition, concepts of process safety, modernization of tannery and process engineering of leather making to identify the need for benign methods in processing have been incorporated. Analysis of life cycle assessment and carbon footprint relevant to leather sector are also provided. This unique and novel review includes 257 references with recent information, leading to environmental protection and process safety. The distinctive approach and analysis presented here provides methodology and novel approach for development of eco-benign alternatives, chemicals and systems for Leather and other generic processing industries for green & sustainable development and also form a typical model for preparedness towards future challenges for sustainable development. This comprehensive analysis and review would pave way for switch over from conventional leather process, which has environmental and safety concerns to alternate eco-benign products, processes and systems.

- **Keywords:** Leather processing; Eco-benign; Process safety; Cleaner production; Sustainable development

Hanan Arahmane, Jonathan Dumazert, Eric Barat, Thomas Dautremer, Frédérick Carrel, Nicolas Dufour, Maugan Michel. *Bayesian inference based on a bivariate gamma distribution of Kibble for low-level radioactivity detection in nuclear decommissioning operations*. Pages 727-742.

Statistical test analysis has proven itself to be versatile tool in various scientific and technical fields, following either a frequentist approach based on a p−value, or a Bayesian approach evaluating a Bayes factor. In this study, the authors adapted a Bayesian approach to a radiation-detection application in the industrial context of nuclear decommissioning. The detection of a weak uranium signal on concrete, under the constraint of a very low signal-to-noise ratio, represents in particular a major challenge in this application area. For this purpose, we developed an original Bayesian statistical hypothesis test based on a bivariate gamma distribution of Kibble. Said test allows merging the absolute and relative characters of two Bayesian tests developed in the same context, as well as providing better performance tradeoff in both cases of stationary and non-stationary radiological backgrounds. The simulation-based study

showed that the proposed Bayesian test should meet the abovementioned expectations, and allow the detection of a relatively low surface activity uranium contamination, while ensuring a competitive tradeoff between statistical sensitivity and specificity.

- **Keywords:** Bayesian inference; Kibble/Dirichlet distributions; Radiation detection; Gamma-ray spectrometry; Nuclear decommissioning