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Wen Shao, Jing Zhu, Zedong Teng, Keyao Zhang, Shuang Liu, Min Li. *Distribution of inorganic phosphorus and its response to the physicochemical characteristics of soil in Yeyahu Wetland, China*. Pages 1-8.

This research investigated spatial and vertical distribution of total phosphorus (TP), inorganic phosphorus (IP) and IP fractions as well as its responses to corresponding physicochemical properties in Yeyahu Wetland. The results shown that TP concentration varied from 335.37 to 683.32 mg kg−1, it was irregularly distributed in horizontal direction but decreased with the soil depth in vertical direction. The IP concentration varied from 249.43 to 387.49 mg kg−1, accounting for 60%–85% of TP. The order of contents were as follows: Ca-P > Fe-P > Ex-P > Al-P > Oc-P. In vertical direction, the Ca-P distributed roughly with IP because Ca-P was found to be the major species (up to 370 mg kg−1). Other forms were found to decrease with soil depth. According to redundancy analysis (RDA), Ex-P was positively correlated to organic matter content (r=0.637, P < 0.001), indicating that organic matter might be of the importance in maintaining P availability in soils. Anew, the TP correlated with the content of soil fine particles (2–20 μm) (r=0.629, P < 0.01), which suggested that fine particles were suitable for P adsorption in soils from Yeyahu Wetland. This study provided data support for sustainable development of wetland ecosystem.

- **Keywords:** Wetland soil; Inorganic phosphorus factions; Spatial distribution; Vertical distribution

Ernesto Rivas, Mónica Calero, Celso Amor, Gabriel Blázquez, Mª Ángeles Martín-Lara, Antonio Pérez. *Mixed solid waste from the decommissioning of coal-fired power plants as a resource of high value metals*. Pages 9-15.

The possibility of recovering metals from a mixture of solid industrial waste generated from decommissioning of a coal-fired power plant has been studied in this work. First, a complete characterization of the material was carried out. Results showed that the material contains an interesting amount of metals (Ti, V, Cr, Ni, Zn and Pb) that can be recovered by acid leaching and chemical precipitation. Then, some leaching tests were performed in batch systems with different acid solutions at different operational conditions. The main effects of leaching time, leaching agent and acidity were investigated. High concentrations of metal were achieved in the leachate obtained when a treatment with sulfuric acid solution at a pH value of 1 was used as leaching agent.

Finally, the metals presented in leaching solution were precipitated by chemical precipitation with NaOH. A good separation of Ti and V respect to the other dissolved elements between pH 4 and 5 was obtained.

- **Keywords:** Chemical precipitation; Coal-fired power plant; Leaching; Metals recovery; Recycling

Zhaoyou Zhu, Xueli Geng, Guoxuan Li, Xiaopeng Yu, Yinglong Wang, Peizhe Cui, Guowu Tang, Jun Gao. *Control comparison of extractive distillation with two different solvents for separating acetone and tetrahydrofuran*. Pages 16-30.

Extractive distillation is a common method to separate the mixture which has the low relative volatility, such as acetone and tetrahydrofuran mixture. Because the number of candidate solvents is high and the experiment is time-consuming, the selection method of solvent is important. In our previous work, quantitative structure property relationship was introduced to model and evaluate the relative volatility of acetone and tetrahydrofuran mixture. The flowsheet of extractive distillation was set up and the total annual cost was calculated with n-Octane and butyl ether as new and former solvent, respectively. Except the mathematical verification, we think that the dynamic control of the configuration of extractive distillation can also be a method to evaluate the feasibility of the built model. In this paper, we studied the dynamic control for extractive distillation with n-Octane and butyl ether as solvent and the integral of squared error was calculated for purity of two products. The results show that some indexes for n-Octane as solvent are better than that for butyl ether as solvent. The dynamic control performance is consistent with the results of economical and can be a way to judge the reliability of quantitative structure property relationship.

- **Keywords:** Process control; Extractive distillation; Quantitative structure property relationship; Modelling and simulation studies

Abbas Jorsaraei Talar, Taghi Ebadi, Reza Maknoon, Alimorad Rashidi. *Investigation on effect of KCl addition on desalination performance of co-polymerized GO/Nylon nanocomposite membrane*. Pages 31-38.

In this research work, following the efforts for providing fresh water for humans, a novel nanocomposite membrane was prepared. In this regard, potassium cation was added to co-polymerized graphene oxide (GO) to tune the interlayer spacing of the GO nanosheets. The prepared membranes were characterized by X-ray diffraction, contact angle measurement, Atomic Force Microscopy (AFM), and Field emission scanning electron microscopy (FE-SEM) equipped with Energy-dispersive X-ray spectroscopy (EDX). The XRD patterns confirmed that by adding potassium chloride (KCl) to GO containing membranes, interlayer spacing was optimized and led to presence of interlayer spacing in the range of 4–6 Å and 7.80 Å which are highly active in rejection of salt ions. To evaluate the desalination performance of the prepared nanocomposite membranes, forward osmosis (FO) process was considered. The results showed that although the membrane showed acceptable permeability, the salt rejection activity was enhanced considerably. The potassium cation containing membrane exhibited reverse salt rejection of 2.03 which was 6.31 in absence of it. This can be attributed to effect of potassium cations in optimizing and modifying interlayer spacing along with repulsion of Na+ due to charge similarity with K+.

- **Keywords:** Modified graphene oxide; Membrane; Forward osmosis; Desalination; Nanocomposite

Saraschandra Naraginti, Yang-Yang Yu, Zhen Fang, Yang-Chun Yong. *Visible light degradation of macrolide antibiotic azithromycin by novel ZrO2/Ag@TiO2 nanorod composite: Transformation pathways and toxicity evaluation*. Pages 39-49.

Macrolide antibiotics are one of the major groups of emerging pharmaceutical contaminants that have been detected in aquatic systems. Photocatalytic degradation under UV light is useful for mineralization of various pharmaceutical pollutants but very limited studies are available for degradation of azithromycin (AZY) using visible light. In the present study, a novel ZrO2/Ag@TiO2 nanorod ternary nanocomposite was prepared by a simple hydrothermal and photodeposition method for efficient degradation of AZY under visible light. The composite was detailed characterized by XRD, XPS and TEM analyses, which revealed the formation of cubic ZrO2 and Ag nanoparticles on TiO2 nanorods (TNR). More than 90% of azithromycin (20 mg/L) was degraded after 8 h of visible light irradiation. The plausible transformation pathway for azithromycin was proposed based on the LC/MS-IT-TOF analysis. The phytotoxicity evaluation of the azithromycin and its degraded products was assessed on Vigna radiata. The germination index (GI) of azithromycin was found to be 12.3% before degradation while it increased to 81.05% after 8 h of degradation, indicating this photodegradation process achieved nearly complete detoxification. Furthermore, the toxicity of the degradation products was determined on the basis of Escherichia coli colony forming unit assay which confirmed high detoxification efficiency. Thus, this work demonstrated an efficient strategy for visible light degradation and detoxification of azithromycin, which provided new insight on macrolide antibiotic photodegradation and would be promising for antibiotic wastewater treatment.

- **Keywords:** Ternary composite; Photodegradation; Macrolide; Visible light; Detoxification

Maja Turk Sekulic, Nikola Boskovic, Aleksandar Slavkovic, Jelena Garunovic, Srdana Kolakovic, Sabolc Pap. *Surface functionalised adsorbent for emerging pharmaceutical removal: Adsorption performance and mechanisms*. Pages 50-63.

A highly effective adsorbent (PPhA) was designed using “acid catalyst” functionalisation and tested for six emerging PhCs (sulfamethoxazole (SMX), carbamazepine (CBZ), ketoprofen (KP), naproxen (NPX), diclofenac (DCF) and ibuprofen (IBF)) in a batch study. Characterisation results (BET, SEM, FTIR, XRD and pHzpc) showed that the functionalisation process generates a microporous material with a multitude of new functional groups (such as phosphate and phosphonate) present on the surface. Adsorption capacity reached near maximum within 10 min while equilibrium was obtained in 60 min. Findings suggest that the mass transfer was governed mainly by intraparticle diffusion processes through formation of H-bonds, π–π and n–π electron donor–acceptor interactions. A pH influence study showed that electrostatic interactions played a minor role in the overall removal mechanism. The magnitude of E was <8 kJ mol−1 for all studied PhCs, indicating that adsorption is mainly due to physisorption. Equilibrium data were best represented by the Freundlich model and the theoretical monolayer adsorption capacities were 17.193, 17.685, 19.265, 17.657, 21.116 and 23.332 mg g−1 for SMX, CBZ, KP, NPX, DCF and IBF, respectively. Based on these results, this PPhA is proposed as an excellent adsorbent for PhC removal.

- **Keywords:** Water management; Functionalisation; Waste recycling; Pharmaceuticals; Adsorption mechanism; Competitive adsorption

Xuelong Lv, Yaqing Zhang, Lin Li, Wenrui Zhang, Peng Liang. *Experimental study of ethanol adsorption using a multistage bubbling fluidized bed*. Pages 64-70.

Adsorption is one of the most efficient inexpensive strategies for the removal of volatile organic compounds (VOCs). However, adsorption of VOCs by fixed beds has certain limitations, such as considerable energy consumption and high operating costs. To treat VOCs with high volume and low concentration, a pilot-scale multistage bubbling fluidized bed adsorber was developed herein and was used to conduct the adsorption experiments. Experimental investigation of ethanol adsorption on the adsorbent under static and dynamic conditions revealed that ethanol adsorption on the adsorbent followed the Langmuir adsorption model. The adsorption kinetics followed a linear driving force (LDF) model, which showed that diffusion was the rate-determining factor. Moreover, the effects of operating conditions, such as bed height, superficial gas velocity, inlet concentration, and desorption temperature, on adsorption were investigated. The results showed that adsorption efficiency in the bubbling fluidized bed varied from 85.7% to 94.5%. The findings of this study could provide the basic data for the design and development of a bubbling fluidized bed for application in the recovery of low-to-medium concentrations of industrial VOCs.

- **Keywords:** VOC adsorption; Activated carbon; Multistage bubbling fluidized bed; Mass transfer

Aliakbar Eslami Baladeh, Morteza Cheraghi, Nima Khakzad. *A multi-objective model to optimal selection of safety measures in oil and gas facilities*. Pages 71-82.

Optimal selection of safety measures (SMs) is a challenging task for safety managers due to its importance, complexity, and incapability of traditional approaches in considering all the aspects of SMs optimal selection. Sophisticated mathematical models can be used to overcome the limitations of traditional approaches. However, setting the objective functions while considering their priorities as well as possible synergistic effects of the SMs on the hazards are still among the main concerns in the development and application of mathematical models. The present study is aimed at developing a methodology to optimize the SMs selection while addressing the aforementioned challenges and considering both the budget and the risks. To do so, first the Pareto set of the solutions is obtained by NSGA-II technique - a multi-objective genetic algorithm technique - where a lexicographic model is used to select the optimal solution from the Pareto set based on the priority of the objective functions. A pessimistic strategy is used to account for the synergistic effects and the overlaps between the selected SMs. Two mathematical models are developed to represent different policies in optimal SMs selection in a gas wellhead and surface facility. The results show a notable difference between the two policies, indicating the importance of setting proper objective functions in multi-objective optimization problems. The results also show that the methodology is able to effectively satisfy different safety management policies and constraints with no need for much extra information except the cost and impact of SMs on the hazards' risk.

- **Keywords:** Safety measures; Lexicographic model; Genetic algorithm; Multi-objective optimization

Bahareh Asefi, Shiue-Lin Li, Henry A. Moreno, Viviana Sanchez-Torres, Anyi Hu, Jiangwei Li, Chang-Ping Yu. *Characterization of electricity production and microbial community of food waste-fed microbial fuel cells*. Pages 83-91.

Food waste (FW) contributes to a great proportion in the municipal solid waste and is generated during disposal from different life cycles of food processing and consumption. FW treatment is a big challenge and there is an urgent need to develop a suitable treatment technology. The microbial fuel cell (MFC) is a promising bioelectrochemical technology using bacteria as the catalyst, which has been developed to effectively generate bioelectricity from diverse organic wastes. The present study investigated the treatment of food waste collected from a Chinese canteen using MFCs under different conditions. It was observed that the highest closed circuit voltage and maximum power density obtained were 775 ± 21 mV and 422 mW m−2, respectively, when using food waste with nutrient medium as the anolyte and permanganate as the catholyte. Under this condition, biodegradation processes in the MFCs could achieve 69 ± 18% COD, 88 ± 5% carbohydrate, 76 ± 9% protein, 65 ± 8% TOC and 71 ± 8% total nitrogen removal. Microbial community analysis using 16S rRNA gene high-throughput sequencing showed Firmicutes, Bacteroidetes and Proteobacteria were the dominant phyla and Geobacter was the most abundant genus. Therefore, our microbial community results suggested that the mixture of exoelectrogenic and fermentative bacteria have a pronounced effect on MFCs system treating FW while affecting on organic degradation and energy production. A power management system was used to demonstrate that electricity from FW-fed MFCs can be successfully harvested to provide intermittent electricity to loads. Overall, this study demonstrated the potential of using MFCs for food waste treatment to achieve electricity production and waste reduction.

- **Keywords:** Food waste; Microbial fuel cell; Permanganate; Ferricyanide; Microbial community; Power management system

Shuaiwei Gu, Yuxing Li, Lin Teng, Cailin Wang, Qihui Hu, Datong Zhang, Xiao Ye, Jinghan Wang, Stefan Iglauer. *An experimental study on the flow characteristics during the leakage of high pressure CO2 pipelines*. Pages 92-101.

High pressure pipeline transportation is dominant mode for economically transporting large amounts of CO2. However, potential leakage is one of the main risks associated with pressurized CO2 pipeline transportation. Thus, to investigate the leakage behavior of high pressure CO2 and to de-risk such transportations, a new laboratory scale experimental setup (total length of 14.85 m and the inner diameter of 15 mm) was constructed. Leakage experiments for pure CO2 and CO2 mixtures containing various N2 concentrations were carried out for different initial phase states (supercritical, liquid and gaseous respectively). The pressure and temperature characteristics and phase transitions of high pressure CO2 were then studied following pipeline leakage through small diameter nozzles. The results show that a minimum temperature occurs during the leakage process of various initial phase states; while the temperature characteristics of supercritical and gaseous CO2 leakage were rather different from that of liquid CO2 leakage. Impacts of impurity (N2), initial inner pressure and nozzle sizes on the leakage behavior were investigated, and two minimum temperature lines, based on N2 concentrations and initial inner pressures were obtained, respectively. These findings will ascertain that the pipeline is operated above the ductile-brittle transition temperature.

- **Keywords:** CO2leakage; Minimum temperature; Phase transition; Brittle fracture; Impurity

Amin Taheri, Ali Taheri, Ali Asghar Fathivand, Nabiollah Mansouri. *Risk assessment of naturally occurring radioactive materials (NORM) in the hydrocarbon sludge extracted from the south pars gas field in Iran*. Pages 102-120.

Natural radionuclides are always present in soil, water, and in particular in materials extracted from the depths of the earth. The accumulation of natural radionuclides and the increase in their radioactivity to excessive levels will lead to health hazards and environmental damages. Therefore, carrying out studies, evaluations and risk assessments in industries with the possibility of excessive accumulation of these materials in their various processes is inevitable to protect occupational health of employees and stakeholders and prevent the pollution of environmental resources including soil, water and air. Oil and gas fields are among the most prepared areas in this regard. Iran is one of the largest owners and producers of huge oil and gas resources in the world. The great concentration of hydrocarbon reservoir extraction and production facilities in some parts of the country, and the presence of a large number of oil & gas organizations employees in these areas, necessitate such studies. For this reason, one of the South Pars gas field refineries located in Pars special economic energy zone, Assaluyeh, Iran, was selected to investigate the concentration of radioactivity of hydrocarbon sludge and soil and the related hazards indices (potential hazards). The obtained results showed that the concentrated sludge in the condensate pre-flash drum of the condensate stabilization unit and some of heat exchangers had higher than normal radioactivity levels. Furthermore, health and environmental risks were assessed and the results indicate that there are high risks in some activities and environmental aspects that it is necessary to consider controls to reduce them to acceptable levels.

- **Keywords:** NORM; Hydrocarbon sludge; Iran; Radiological parameters; Gas field; Risk assessment; Health hazard; Environmental hazards

Finella Jianna A. Villaluz, Mark Daniel G. de Luna, James I. Colades, Sergi Garcia-Segura, Ming-Chun Lu. *Removal of 4-chlorophenol by visible-light photocatalysis using ammonium iron(II) sulfate-doped nano-titania*. Pages 121-128.

Halogenated aromatic compounds are toxic and carcinogenic. This is the case of 4-chlorophenol (4-CP), a priority pollutant found in large amounts in industrial wastewater effluents from pharmaceutical, dye, pulp and paper industries. Long term exposure to 4-CP even at low-concentration is associated to endocrine disruption. Photocatalysis is a promising advanced oxidation process that attains complete degradation of organic pollutants. The use of UV lamps undermines actual photocatalysis application due to the electrical energy requirements. In this frame, the development of visible light photoactive catalysts can overcome these challenges allowing the implementation using affordable light sources like light emitting diodes (LEDs) or natural sunlight. This work is to present the synthesis and use of an alternative photocatalyst that provided eight-fold increase on 4-CP degradation in comparison to commercial TiO2 Degussa P-25. Almost complete removal (99.20%) was achieved with synthesized Fe/N/S-doped TiO2 at 1.0 g L−1 of photocatalyst dose and pH 7.0 for treating 10 ppm of 4-CP.The first-order rate constant, kLH, and Langmuir adsorption constant, KLH, were calculated with values of 0.429 min−1 and 2.326 ppm−1, respectively. The Fe/N/S-TiO2. photocatalysts showed an excellent stability maintaining their performance during four cycles of recovery/reuse.

- **Keywords:** Persistent organic pollutants; Wastewater treatment; Visible light photocatalyst; Nanotechnology; Advanced oxidation process

Bartłomiej Hernik, Wiesław Zabłocki, Olgierd Żelazko, Grzegorz Latacz. *Numerical research on the impact of changes in the configuration and the location of the over fire air nozzles on the combustion process in the ultra-supercritical BP 680 boiler*. Pages 129-142.

Primary methods of reduction of nitrogen oxides compared to secondary ones are definitely cheaper in construction and operation, therefore they are still being developed.

They are the first step in the reduction of nitrogen oxides and the basis for the use of more advanced methods. The paper presents the innovative research results of the multivariate numerical calculations on the combustion process supported by zero-dimensional calculations of the novel ultra-supercritical boiler BP-680. The numerical model was verified based on the boiler design calculations, made using the advanced 0-dimensional model of the whole boiler. The calculations were carried out in Ansys Fluent Workbench. On the basis of the obtained results, the effect of changing the configuration and the location of OFA nozzles on flue gas temperature, CO, O2 and NOx content in the flue gas, the heat flux along the height of the furnace chamber, and the burnout in the slag hopper and fly ash were analysed. It is very important in the boiler design process the numerical analysis of the impact of the location and the configuration of OFA nozzles on the combustion process. The results of calculations included in this work will help the boiler designer to create a product that is environmentally friendly.

- **Keywords:** Numerical simulations; Ultra-supercritical boiler; Coal combustion; Furnace chamber; Air staging

Narasamma Nippatla, Ligy Philip. *Electrocoagulation-floatation assisted pulsed power plasma technology for the complete mineralization of potentially toxic dyes and real textile wastewater*. Pages 143-156.

In this study, experiments were conducted for the treatment of textile wastewater containing- a diazo dye i.e. Congo Red dye (CR) and a basic dye Methylene Blue (MB). Performances of Electrocoagulation-Flotation (EC-F) and Pulsed Power Plasma Treatment (PPT) technologies were evaluated individually and in combination. The effects of various parameters such as electrolysis time, electrical conductivity (EC, mS/cm), current density (mA/cm2) and initial concentrations of dye were experimentally optimized to get high removal efficiency. Using EC-F alone, the dye concentration was reduced from 50 mg/L to BDL (below detection level) and 50 mg/L to 3.1 mg/L for CR and MB dyes, respectively at a current density of 14.2 mA/cm2, electrical conductivity 8 mS/cm. To achieve this, an electrolysis time of 2 and 14 min were employed for CR and MB, respectively. To mitigate the problems of passivation of electrodes and sludge formation, EC-F was integrated with PPT treatment system. Also, the removal efficiencies of both the systems were evaluated by treating mixed dyes and real textile wastewater. It was found that by giving a partial treatment in EC-F followed by PPT was able to achieve 100% (TOC) degradation of MB with a total energy consumption of 50.55 kW h/kg dye removed and 39.3 kW h/kg dye for CR. The complete (100%) mineralization of the pollutant was achieved without any chemical addition and no waste (sludge) was produced at the end of novel hybrid treatment. The total treatment cost was reduced by 41.2% (86.04 kW h/kg dye to 50.55 kW h/kg dye) for MB and 30.7% (56.7 kW h/kg dye to 39.3 kW h/kg dye) for CR in hybrid system as compared to PPT treatment alone. Hybrid treatment was found to be an economical and a reliable technology for treating textile industry wastewater.

- **Keywords:** Electrocoagulation-flotation; Pulsed power technology; Hybrid system; Methylene blue (MB); Congo red (CR); Cationic; Anionic

Dmitry Sofronov, Alla Krasnopyorova, Natalya Efimova, Anna Oreshina, Ekaterina Bryleva, Galina Yuhno, Sergiy Lavrynenko, Miroslaw Rucki. *Extraction of radionuclides of cerium, europium, cobalt and strontium with Mn3O4, MnO2, and MNOOH sorbents*. Pages 157-163.

The paper describes the tests carried out for the extraction of radionuclides 90Sr, 137Cs and 60Co by manganese oxyhydroxide in order to compare the sorption properties of the respective particles with Sr(II), Co(II), Ce (III), Eu (III) ions. It was found that the recovery efficiency and the sorption capacity with respect to metal ions decrease in the MnOOH → MnO2 → Mn3O4 series. The tests proved that the extraction of the

radionuclides from tap water by MnOOH particles was 53.7%, 83.5% and 93.1%, respectively.

- **Keywords:** Extraction; Adsorption; Cobalt; Cesium; Strontium; Radionuclides; Manganese oxyhydroxide

Aitao Zhou, Lingpeng Fan, Kai Wang, Derek Elsworth. *Multiscale modeling of shock wave propagation induced by coal and gas outbursts*. Pages 164-171.

We explore the propagation modes of shock waves driven by coal and gas outbursts in both the near- and far-field. Near-field response is three-dimensional (3D) at the face, but the far-field is constrained to one-dimensional (1D) flow within the roadways. Fluent models are applied to simulate the 3D propagation of shock waves at the outburst source with 1D models utilizing Flowmaster being sufficient distal from the face. These models are linked via a Mesh-based parallel Code Coupling Interface (MPCCI) to define shock wave propagation at all scales – from mine face to distal roadways. The results demonstrate the suitability and fidelity of the Flowmaster 1D simulation in representing the time history of overpressure. The shock wave attenuation in each part of the MPCCI coupled model is consistent with experimental results. This work provides a logical, consistent and robust method to solve for the complex coupling at multiple length- and time-scales and its implementation as an "outburst" pipe network. Additionally, it has significant utility in designing for outburst mitigation, disaster ventilation and other safety measures.

- **Keywords:** Coal and gas outburst; Shock wave propagation; Multiscale coupling; Flowmaster; MPCCI coupling

Satya Sundar Mohanty, Hara Mohan Jena. *Degradation kinetics and mechanistic study on herbicide bioremediation using hyper butachlor-tolerant Pseudomonas putida G3*. Pages 172-181.

The present study reports a new bacterial isolate identified as Pseudomonas putida strain G3 that can be used for the efficient biodegradation of butachlor, a systemic selective herbicide. Reports suggests butachlor to be a persistent pollutant, a suspected carcinogen and mutagen which poses threat to the environment. Batch biodegradation of the herbicides over a concentration ranging from 100 to 1000 mg/L by the bacterial strain has been studied after process parameter optimization. The bacterial strain is able to degrade up to 700 mg/L of butachlor completely within 360 h. However, increasing the concentration of the herbicide resulted in substrate inhibition in the efficiency of the microbial strain G3. Thus, to determine the bio-kinetic parameters, various inhibition models were fitted to the results obtained during batch biodegradation study. The maximum estimated specific degradation rate was found to be 2.74 mg/L/h. To enhance the bioremediation efficiency of the bacterial strain in presence of higher concentration of the herbicide, the microbial cells were immobilized on Ca-alginate beads and the efficiencies of free and immobilized bacterial cultures were evaluated. The ESI-MS analysis indicated that butachlor biodegradation took place with 2-chloro-N-(2,6-diethylphenyl)-N-hydroxymethylacetamide, 2-chloro-N-(2,6-diethylphenyl) acetamide and 2,6-diethylaniline as intermediate metabolites and a degradation pathway has been proposed. The bacterial strain is able to degrade up to 500 mg/L and 1000 mg/L of other herbicides such as Alachlor and Glyphosate efficiently proposing its wide substrate specificity. The study serves as an important basis that should help to design future bioremediation technology that would be expedient for the treatment of various herbicides.

- **Keywords:** Butachlor; Bioremediation; Environmental pollution; Immobilization; Metabolites

Jih-Hsing Chang, Shui-Wen Chang Chien, Cheng-Di Dong, Chiu-Wen Chen, Chien-Hung Huang, Shan-Yi Shen. *The coinage refractory wastewater treated by electrocatalytic-membrane process (ECMP) integrated with chemical- or electro-coagulation techniques*. Pages 182-188.

Some industrial wastewater containing complicated contents (e.g., heavy metals and organics) and extensive concentration-variation cannot be well-treated by physical-chemical treatment processes. In order to obtain the feasible electrochemical technique, an electrocatalytic-membrane process (ECMP) was established to treat such wastewater from a mint factory in Taiwan. Wastewater samples with pollutants of Cu2+, Ni2+ and chemical oxygen demand (COD) were categorized into three types based on pH and concentrations. The complexity of wastewater is attributed that a verity of chemical reagents and manufacturing methods are employed to produce different kind of coins. In this study, each type of wastewater was treated by the ECMP and integrated with other techniques to find out the appropriate procedures. Results indicate that the sole ECMP can effectively remove the Cu2+, Ni2+, and COD when the wastewater is with relatively low pH (around 3–5), low COD (around 50 mg L−1), and high concentration of heavy metals (Cu2+ concentration over 500 mg L−1). However, the ECMP should combine with pH-adjustment to effectively remove the Cu2+, Ni2+, and COD when the wastewater is with very low pH (close to 1), high COD (over 200 mg L−1), and high concentration of heavy metals. In addition, the ECMP has to link the electrocoagulation (ECG) to decrease the Cu2+, Ni2+, and COD concentration when the wastewater is with neutral pH (around 7), middle-level COD (around 130 mg L−1), and low concentration of heavy metals (Cu2+ concentration around 1.0 mg L−1). Accordingly, the ECMP integrated with other treatment processes gains potential to treat refractory wastewater.

- **Keywords:** COD; Electrocatalytic; Electrocoagulation; Heavy metals; Industrial wastewater

Yu Han, Zhenwu Tang, Jiazheng Sun, Xiangyang Xing, Minna Zhang, Jiali Cheng. *Heavy metals in soil contaminated through e-waste processing activities in a recycling area: Implications for risk management*. Pages 189-196.

Heavy metal pollution of the environment caused by e-waste recycling is of increasing concern, but little information is available on metal emissions during e-waste processing activities. Here, the concentrations of nine metals in soil at four contaminated sites in Qingyuan (an e-waste recycling area in China) and the risks posed were investigated. Soil at the sites was polluted with metals, particularly Cd, Cu, Pb, and Sb, the concentrations of which were 2.83–2306, 2.17–1880, 0.96–1971, and 9.28–5607 times higher, respectively, than local background concentrations. The Cd, Cr, Hg, Pb, and Sb concentrations were significantly lower in soil at an abandoned site than at acid-leaching, dismantling, and burning sites. The risks posed by metals in soil to human and environmental health were much higher at the acid-leaching and burning sites than the dismantling and abandoned sites. Source assessments indicated the differences in metal concentrations at the different sites were caused by different e-waste recycling activities at the sites. The results indicated crude e-waste processing is an important source of heavy metals to soil and should be of great concern. Pollution control measures and risk management strategies specific to soil contaminated through e-waste processing activities should be developed.

- **Keywords:** E-waste recycling site; Heavy metals; Ecological risks; Human health risks; Differences

Fengxian Fan, Sihong Zhang, Wenying Wang, Jinpei Yan, Mingxu Su. *Numerical investigation of PM2.5 size enlargement by heterogeneous condensation for particulate abatement*. Pages 197-206.

Vapor heterogeneous condensation with PM2.5 as nuclei is a promising approach to enlarge the particle sizes and thus facilitate subsequent particulate abatement by the existing inertial separators. However, the investigation on PM2.5 size enlargement by vapor heterogeneous condensation, which is important to optimize the particulate abatement process, has been largely lacking. In this study, the evolution of particle size distribution due to vapor heterogeneous condensation on the surfaces of polydisperse insoluble PM2.5 was modelled based on the classical heterogeneous nucleation theory and the condensation droplet growth theory. Using this model, the effects of operational parameters on the particle size distribution after heterogeneous condensation were numerically investigated. The results show that the polydisperse fine particles shift to monodisperse coarse particles at a small contact angle, whereas bimodal particle size distribution after heterogeneous condensation is generated at a large contact angle. Higher vapor saturation ratio, higher gas temperature, longer residence time, and greater geometric mean particle size are beneficial to PM2.5 size enlargement and subsequent particulate abatement. Moreover, the geometric standard deviation of particle sizes has little effect on the PM2.5 size enlargement. The model predictions of the particle size distribution after vapor heterogeneous condensation match well with the experimental data.

- **Keywords:** PM2.5; Heterogeneous nucleation; Condensation growth; Particle size enlargement; Particulate abatement; Numerical simulation

Shuailong Li, Gang Zhou, Yuying Wang, Bin Jing, Yalong Qu. *Synthesis and characteristics of fire extinguishing gel with high water absorption for coal mines*. Pages 207-218.

Coal mine fires pose a threat to the lives of underground workers and cause incalculable losses to the national economy. When a fire occurs, the temperature in the underground wells will rise, which becomes a huge hidden danger that needs to be controlled to prevent disasters. In this paper, using sodium carboxymethyl cellulose as a matrix and through graft copolymerization of acrylic acid and 2-acrylamide-2-methylpropanesulfonic acid, a novel fire-extinguishing gel with high water absorption and high resistance has been prepared. It has a high water absorption ratio as well as an excellent fire prevention effect. The microscopic reaction and structure of the product are analyzed by infrared spectroscopy, thermogravimetry, X-ray diffraction and scanning electron microscopy. By testing the properties of the gel, it is proven that the product has a fast water absorption rate with a high ratio, strong salt tolerance, good water retention and the obvious effects of filling, sealing and fire extinguishing.

- **Keywords:** Sodium carboxymethyl cellulose; 2-Acrylamide-2-methylpropanesulfonic acid; Coal mine fire; High water absorption and high resistance; Fire-extinguishing gel

Cheng-Di Dong, Yung-Chi Lu, Jih-Hsing Chang, Tsing-Hai Wang, Chiu-Wen Chen, Chang-Mao Hung. *Enhanced persulfate degradation of PAH-contaminated sediments using magnetic carbon microspheres as the catalyst substrate*. Pages 219-227.

The advanced oxidation process (AOP) is a promising remediation technology for persistent organic pollutants in the environment. We herein investigated the ability of a magnetic carbon microsphere (CM)-based composite catalyst (Fe3O4−CM) to catalyze sodium persulfate (Na2S2O8, SPS) for the remediation of marine sediments

contaminated with polycyclic aromatic hydrocarbons (PAHs). The effectiveness of the process parameters, catalyst dose, and initial pH were investigated. Using the optimized conditions, 87% of the PAHs were removed in the Fe3O4−CM/PS system within 24 h, compared with 59% and 41% in the case of persulfate (PS) and CM/PS (PS concentration = 1.3 × 10−5 M, catalyst concentration = 5.0 g/L, pH = 6.0) alone. The PAH reduction rate can be attributed to the uniform graphitic structure of Fe3O4−CM, which serves as an effective matrix for PAH degradation by providing additional active sites. The degradation of the PAHs was related to the number of rings in their structure, as confirmed by the higher degradation efficiency observed for high aromatic ring PAHs (HPAHs). Thus, we herein demonstrated the CM-mediated electron transfer catalysis of the surface functional groups at circumneutral pH values in the Fe3O4−CM/PS system to the highly efficient removal of PAHs from contaminated sediments.

- **Keywords:** Carbon microspheres; Polycyclic aromatic hydrocarbons; Sediment; Remediation

Pengfei Wang, Chang Tian, Ronghua Liu, Jian Wang. *Mathematical model for multivariate nonlinear prediction of SMD of X-type swirl pressure nozzles*. Pages 228-237.

X-type swirl pressure nozzle is a new type of nozzle with the spin core structure. Due to its superior atomization characteristics, it has been widely applied in the field of spraying dust suppression in recent years. Sauter mean diameter (hereinafter referred to as SMD) is an important indicator to evaluate the atomization characteristics and dust suppression performance of nozzles. In order to build the SMD prediction model for this type of nozzles, based on the independently designed spray experiment platform, the interaction law between the nozzle SMD and the four influence factors is obtained through the orthogonal design method. On this basis, a mathematical model for predicting the nozzle SMD is built using the multivariate nonlinear regression method. The results show that SMD increases with the increase of axial distance, absolute radial distance value and nozzle diameter, but decreases with the increase of feed water pressure. The primary and secondary sequence of the four factors affecting SMD is: feed water pressure > axial distance > nozzle diameter > radial distance. The fitting values of the multivariate nonlinear regression model are basically the same with the experimental values, with the relative error of less than 3.50% and the average relative error of only 1.35%, which can be used for the theoretical calculation of the SMD of the X-type swirl pressure nozzles. The multivariate nonlinear prediction model built in this study can provide guidance for the design and selection of such spraying dust suppression schemes as nozzle outlet diameter, feed water pressure and nozzle layout, etc. for the field engineering application of such nozzles.

- **Keywords:** X-type swirl pressure nozzle; Sauter mean diameter (SMD); Rthogonal experiment; Ultivariate nonlinear; Rediction model

Esrafil Asgari, Ali Esrafili, Roohollah Rostami, Mahdi Farzadkia. *O3, O3/UV and O3/UV/ZnO for abatement of parabens in aqueous solutions: Effect of operational parameters and mineralization/biodegradability improvement*. Pages 238-250.

Methyl-, Ethyl-, Propyl-, Butyl-, & Benzyl-paraben degradation is investigated by combination of ZnO-based photo-catalysis and ozonation in a batch cylindrical photo-reactor to evaluate the influence of ZnO concentration, ozone dose, and pH. The results reveal that parabens removal increases by rising the ozone dosage up to 1.8 g/h and ZnO loading climb up to 1 g/L. Optimum pH value for parabens removal is 9, in 1 g/L of ZnO and 1.1 g/h of ozone dose in 20 min reaction time, which leads to complete removal of methyl-paraben by the combined photocatalytic ozonation (O3/UV/ZnO).

- **Keywords:** Endocrine disrupting compounds (EDCs); Parabens; Photocatalytic ozonation; Synergistic effect; Water pollution; ZnO

Peitao Su, Jiajie He, Xingtao Zuo, Zhongbing Chen, Zhenhua Li. *Modelling the simultaneous effects of organic carbon and ammonium on two-step nitrification within a downward flow biofilm reactor*. Pages 251-259.

Process modelling is an approximated description of the reality, and choosing appropriate kinetics forms is crucial for model accuracy. It has been long observed that the inhibition effect from organic carbon on nitrification does not change gradually as the organic carbon level changes, which is not capable to be adequately reflected by traditional Monod type kinetics. Therefore, with a purpose to address this issue from modelling perspectives, this study combines the inhibition effects from organic carbon and ammonium on two-step nitrification and incorporates them into a modified ASM1 (Activated Sludge Model No.1) based two-step nitrification framework using two different forms: one in traditional Monod type and one in Logistic type. The two modified models demonstrate improvements in model prediction from both temporal and spatial perspectives, with the Logistic type model even better than the Monod type model. Simulated bacterial depth profiles of the biofilm reactor correspond to lab observations in that heterotrophs dominate the upstream layers where nitrification is inhibited, while ammonia-oxidizing bacteria (AOB) and nitrite-oxidizing bacteria (NOB) dominate the downstream layers where the inhibition on nitrification is relieved. A direct implication for process control is that higher media porosity and longer biofilm length can work in favor of nitrification, but higher hydraulic loadings and higher ratio of organic carbon over ammonium in the influent will be undesirable for nitrification. Overall, a necessity is proven in this study to use appropriate numerical forms to describe the combined inhibition effects of organic carbon and ammonium on two-step nitrification.

- **Keywords:** AQUASIM; ASM; Biofilm reactor; Modelling; Partial nitrification

Juan Du, Lei Zhang, Amjad Ali, Ronghua Li, Ran Xiao, Di Guo, Xiangyu Liu, Ziyang Zhang, Chunyan Ren, Zengqiang Zhang. *Research on thermal disposal of phytoremediation plant waste: Stability of potentially toxic metals (PTMs) and oxidation resistance of biochars*. Pages 260-268.

Thermal conversion of phytoremediation plant waste into biochar was performed as a safe approach for organic waste management. In this work, a promising phytoremediation plant—Silphium perfoliatum L. was pyrolyzed for biochar production at 350, 550 and 750 °C. The long-term leaching risk of potentially toxic metals (PTMs) in the derived biochars and the oxidation resistance of the biochars were investigated. The results showed that PTMs in the biochar could transform into more stable and less toxic forms with the elevated pyrolysis temperature. PTMs leaching behavior in the 350 °C biochar was considerably sensitive to the leaching while that in the 750 °C biochar was not affected. The biochar produced at a higher temperature possessed a greater oxidation resistance with little amount of C loss, and the stronger oxidation resistance would prevent the release of metals bound to the organic matter. The findings of this study demonstrated that high-temperature pyrolysis was able to reduce the potential risk of PTMs and ensure carbon stability.

- **Keywords:** Plant waste; Biochar; Potentially toxic metals (PTMs); Long-term leachability; Oxidation resistance

Lin-Yong Cui, Wei-Min Ye, Qiong Wang, Yong-Gui Chen, Bao Chen, Yu-Jun Cui. *Investigation on gas migration in saturated bentonite using the residual capillary pressure technique with consideration of temperature*. Pages 269-278.

Determination of parameters for description of gas migration in saturated bentonite is of great importance for the design and construction of artificial barriers in the geological repository for the disposal of high-level radioactive nuclear waste. In this paper, temperature-controlled gas injection tests were conducted on initially water-saturated bentonite specimens using the residual capillary pressure (RCP) technique. Effective gas permeabilities in low injection pressures and the gas breakthrough pressures at temperatures 20, 40 and 60°C were obtained. Results show that: (i) for all the temperatures tested, the intrinsic water permeabilities (kin) range between $3.2 \times 10-20$ and $5.72 \times 10-20$ m2, furthermore, those values increase with rising temperature. Meanwhile, the intrinsic water permeabilities derived from the steady state tests are lower than those obtained from the non-steady state tests; (ii) for all the temperatures tested, the effective gas permeabilities (keff) corresponding to the viscous gas flow before gas breakthrough range between 4.81×10-24 and 2.74×10-22 m2, with slight fluctuations with time. The maximum effective gas permeabilities measured at the occurrence of gas breakthrough on the initially water-saturated bentonite specimens extend from 2.27×10-18 up to 3.32×10-17 m2 and increase as temperature increases, while the time required for gas breakthrough decreases as temperature increases; (iii) for all the temperatures tested, the gas breakthrough pressures measured on the initially water-saturated bentonite specimens vary from 2.74 to 4.08 MPa, while the residual capillary pressure differences, also denoted as snap-off pressures (Psnap-off), range from 0.2 to 0.38 MPa. Additionally, the gas breakthrough pressures and the residual capillary pressures decrease as temperature increases.

- **Keywords:** GMZ bentonite; Temperature; Effective gas permeability; Gas breakthrough pressure; The RCP technique

V. Kavitha, V. Geetha, P. Jennita Jacqueline. *Production of biodiesel from dairy waste scum using eggshell waste*. Pages 279-287.

An effluent from the dairy industry, waste scum oil containing triglycerides of fatty acids from C4- C18 was selected as a potential feedstock for biodiesel production in the presence of nano calcium oxide obtained from modified eggshell. The eggshell waste was calcined at 800 °C to facile synthesize nano calcium oxide and was characterized by X-ray diffractometer (XRD), Fourier Transform Infrared spectrometer (FTIR) and Scanning Electron Microscope (SEM). The calcined eggshell contains mainly nano calcium oxide (CaO) in calcite form with the crystallite size ranging from 16 to 22 nm. The transesterification reaction was carried out in a batch reactor and the operating parameters like catalyst loading, the molar ratio of methanol: oil, reaction temperature and time were optimized. Maximum biodiesel yield of 96% was obtained at the molar ratio of methanol: oil of 6:1, catalyst amount of 2.4 wt% and the reaction temperature of 65 °C for 3 h. The quality of biodiesel produced by transesterification of dairy waste scum was tested on variable four-stroke compressible diesel engine and found to be comparable with conventional diesel in brake thermal efficiency and specific fuel consumption. The biodiesel produced possessed high cetane number and low NOx, than conventional diesel. The results proved that nano CaO obtained from eggshell can be effectively reused and recycled as a heterogeneous catalyst for biodiesel production.

- **Keywords:** Dairy waste scum; Eggshell; Transesterification; Engine performance; Exhaust gas

F. Parrino, S.F. Corsino, M. Bellardita, V. Loddo, L. Palmisano, M. Torregrossa, G. Viviani. *Sequential biological and photocatalysis based treatments for shipboard slop purification: A pilot plant investigation*. Pages 288-296.

This study investigated the treatment of a shipboard slop containing commercial gasoline in a pilot plant scale consisting of a membrane biological reactor (MBR) and

photocatalytic reactor (PCR) acting in series. The MBR contributed for approximately 70% to the overall slop purification. More precisely, the biological process was able to remove approximately 40%, on average, of the organic pollution in the slop. Nevertheless, the membrane was capable to retain a large amount of organic molecules within the system, amounting for a further 30% of the influent total organic content removal. However, this affected the membrane fouling, thus resulting in the increase of the pore blocking mechanism that accounted for approximately 20% to the total resistance to filtration ($2.85 \cdot 1013\ m^{-1}$), even if a significant restoration of the original membrane permeability was obtained after chemical cleanings. On the other hand, the biological treatment produced a clear solution for the photocatalytic system, thereby optimizing the light penetration and generation of highly oxidizing active oxygen species that enabled the degradation of bio-recalcitrant compounds. Indeed, low total organic carbon (TOC) values ($<10\ mg\ L^{-1}$) were achieved in the output of the photocatalytic reactor by means of only 60 Einstein (E) of cumulative impinging energy after the addition of $K_2S_2O_8$. Overall, coupling the two processes enabled very high TOC removal (ca. 95%).

- **Keywords:** Integrated AOPs; Photocatalysis; MBR; Saline wastewater; Slop

Min Li, Deming Wang, He Shan. *Risk assessment of mine ignition sources using fuzzy Bayesian network*. Pages 297-306.

The types of ignition sources in coal mines have complicated diversity and susceptibility due to the environmental complexity in the coal mine production process. To determine the actual ignition cause of a potential accident scene and prevent the occurrence of gas explosions, this work provides a new risk analysis method for mine ignition source based on the fuzzy Bayesian network (FBN). The first step relates to risk factor analysis and the BN model establishment. In light of the expert group decision-making method, risk topological structural models of ignition sources are constructed. The second step is fuzzification and defuzzification. To ensure the reliability of data in the process of expert investigation, this study proposes to calculate the weights of experts using a fuzzy analytic hierarchy process (FAHP) method based on subjective and objective expert weights. The last step uses causal reasoning, logical reasoning and sensitivity analysis to calculate the probability of occurrence of potential risk events and the probability distribution of risk factors. Through the case study of Babao Coal Mine in China, it is demonstrated that the FBN simulation provides a feasible method for accurately identifying the cause of gas explosion ignition. The proposed model can be used by analysts and decision-makers in the coal mine as a decision support tool to increase the probability of the ignition source in complex environments.

- **Keywords:** Ignition source; Coal mine; Fuzzy Bayesian network; Sensitivity analysis

Jie Yu, Dingshun Wang, Zhao Zeng, Lushi Sun. *Experimental research on denitrification and elemental mercury removal by Surface Dielectric Barrier Discharge*. Pages 307-316.

A spiral Surface Dielectric Barrier Discharge reactor was employed to remove both NO and Hg from the flue gas. The effects of O_2 and peak voltage were extensively studied. Only NO, NO_2 and N_2O were observed using FTIR at the outlet of the reactor in the atmosphere of $NO/O_2/N_2$. A desired NO conversion efficiency of 99.2% at 7 kV was obtained in the absence of O_2 with low energy cost. The presence of O_2 can suppress the reduction reaction while accelerating the oxidization of NO, consequently restraining the NO reduction to N_2 and promoting the NO_2 generation. O_2 is necessary for the oxidation of Hg. At peak voltage of 7.0 kV, the Hg conversion reached above 94% at O_2 concentration higher than 4%. It decreased to lower than 55% at 3.5 kV. Different concentrations of CO_2, C_2H_4, SO_2, HCl and H_2O were also introduced to study their effect on NO and Hg conversions. When the CO_2 concentration was increased from 0% to

5 and 10%, the NO conversion decreased from 81.0% to 74.1% and 73.6% respectively. At peak voltage of 7 kV and 500 ppm and 1000 ppm of C2H4 were introduced, the NO conversion increased from 78.7% to 85.4% and 93.8% accordingly, while Hg removal efficiency declined. With HCl concentration increasing to 30 and 60 ppm, the Hg oxidation rate increased significantly to above 90% at peak voltage of 9 kV. A strong inhibition effect of SO2 and H2O on NO and Hg conversion were observed.

- **Keywords:** Surface Dielectric Barrier Discharge; NOx; Hg; Gas component

Lluís Godo-Pla, Pere Emiliano, Fernando Valero, Manel Poch, Gürkan Sin, Hèctor Monclús. *Predicting the oxidant demand in full-scale drinking water treatment using an artificial neural network: Uncertainty and sensitivity analysis*. Pages 317-327.

Drinking Water Treatment Plants face changes in raw water quality and quantity and the treatment needs to be adjusted accordingly to produce the best water quality at the minimum environmental cost. The amount of data generated along drinking water treatment plants allows developing data-based models like artificial neural networks that are able to predict operational parameters and can be incorporated into environmental decision support systems. In the present study, an artificial neural network is developed for predicting the potassium permanganate demand at the inlet of a full-scale Drinking Water Treatment Plant. A systematic methodology is carried out for outlier detection and removal from the original dataset. Afterwards, model parameters estimation, uncertainty and sensitivity analysis is reported to assess prediction quality and uncertainty of the models. Bootstrap method was used for parameter estimation, and uncertainty of the inputs onto the model outputs was propagated using a Monte Carlo scheme. Several sensitivity analysis methods were evaluated to understand the contribution of the inputs on the output of the models, and this was in accordance with the knowledge of the process and other studies found in the literature. The selected architecture consisted of a feed-forward multi-layer perceptron with four inputs and one node in the hidden layer with a sigmoid activation function. The mean absolute error of the resulting model is 0.128 mg·L−1, which was considered acceptable by the DWTP operators. The resulting model provided good results in terms of replicative, predictive and structural performance and is to be used for supporting decision-making in the daily operation of the plant.

- **Keywords:** Artificial neural network; Uncertainty; Sensitivity; Water treatment; Oxidation; Permanganate

Tatiana Kasperski, Olga Kuchinskaya, Paul Josephson. *Response to Waddington et al. on "J-value assessment of relocation measures following the nuclear power plant accidents at Chernobyl and Fukushima Daiichi"*. Pages 331-333.

This is a response to Waddington et al. who argue that there was insufficient public health benefit to justify the relocation of several hundred thousand individuals after the Chernobyl and perhaps Fukushima nuclear accidents. We believe the arguments are not defensible either from a radiological/public health point of view, or from a consideration of costs, and we are skeptical of the use of the "J-value assessment" as a foundation to reach these conclusions. There is debate about the health consequences of exposure to ionizing radiation; data on health impacts are often uncertain and incomplete, and therefore not the basis on which to hesitate to evacuate those affected.

- **Keywords:** Chernobyl; Fukushima; Nuclear accident; Evacuation; Ionizing radiation

Ming Lei, Lin Tang, Huihui Du, Liang Peng, Baiqing Tie, Paul N Williams, Guoxin Sun. *Safety assessment and application of iron and manganese ore tailings for the remediation of As-contaminated soil*. Pages 334-341.

Iron ore tailings (FeT) and manganese ore tailings (MnT), which are abundant and inexpensive materials that contain many trace elements, were employed for the remediation of As-contaminated soil to mitigate As accumulation in rice under greenhouse conditions. Prior to the experiments, the toxicities of both amendments were assessed with the toxicity characteristic leaching procedure (TCLP) and horizontal vibration method (HVM). Based on the assessment results, both amendments were pretreated until no As was present in the leaching solution. After application of both amendments to the soil, the soil pH increased significantly ($p < 0.05$). The ranges of As concentrations in husk and brown rice samples were 0.13–1.54 mg kg−1 and 0.06–0.42 mg kg−1, respectively. The lowest concentrations of As (0.06±0.02 mg kg−1) in rice grains were observed with MnT treatment, which was related to the structure and composition of MnT. There was a significant negative relationship ($p < 0.05$) between Mn and As in rice plants, while there was a significant positive relationship ($p < 0.05$) between Fe and As in rice plants as well as the ratio of Fe/Mn and As in rice plants. In conclusion, MnT could potentially be useful as an amendment to remediate As-contaminated soil and control As uptake by rice plants.

- **Keywords:** Toxicity assessment; Iron ore tailing; Manganese ore tailing; As-contaminated soil; Rice plant; Remediation

Francesco Maluta, Alessandro Paglianti, Giuseppina Montante. *Modelling of biohydrogen production in stirred fermenters by Computational Fluid Dynamics*. Pages 342-357.

A bioreactor for the production of hydrogen from the dark fermentation of organics is studied by a comprehensive modelling strategy. The bioreactor is a dual impeller vortex ingesting stirred tank working under batch and attached-growth conditions. Two geometrical configurations of the reactor are investigated: one devised to ensure an effective fluid dynamics behaviour and the other proposed to increase the hydrogen productivity. The turbulent gas–liquid fluid dynamics, the production and the recovery of H2 from the liquid phase are predicted by the numerical solution of the two-phase Reynolds averaged Navier–Stokes equations and the species mass transport equations, including a simplified kinetic model for the fermentative hydrogen production found in literature and a local interphase mass transfer model for the hydrogen stripping from the aqueous to the gas phase. A simplified model for the description of the interfacial area in the context of the two-fluid model is also proposed. This work suggests a method for the predictive simulations of a complex biological process via numerical modelling based on Computational Fluid Dynamics. The main outcome of the proposed investigation method is a detailed estimation of the different relevant variables and their interaction on a local basis, providing a viable tool for the optimization and the scale-up of bioreactors.

- **Keywords:** Biohydrogen; CFD; Bioreactors; Fermentation kinetics; Interphase mass transfer