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Engy Ahmed, Hesham M. Abdulla, Amr H. Mohamed, Ahmed D. El-Bassuony. *Remediation and recycling of chromium from tannery wastewater using combined chemical–biological treatment system*. Pages 1-10.

Tannery wastewater containing chromium (Cr) is one of the most serious problems in leather industry. In order to develop an effective and eco-friendly treatment technology, a combined chemical–biological treatment system was performed for Cr remediation and recycling. The aim of the present study is to design a laboratory scale system using chemical precipitation of Cr(III) combined with biological removal of Cr(VI) from tannery wastewater, and to investigate the possibility of recycling the recovered Cr(III) in the tanning industry. Chemical precipitation of Cr(III) was carried out using lime and cement dust. The actinomycete strain Kitasatosporia sp. was used in microcosm studies for Cr(VI) bioremoval. Moreover, parameters such as type of porous medium, inoculum size, flow rate and culture conditions were investigated. The precipitated Cr(III) that was recovered from the chemical precipitation stage was recycled in the leather tanning industry. Our findings indicate that the maximum Cr(III) precipitation (98%) was achieved using 2 g/100 mL of lime and 2 h of settling rate. On the other hand, microcosm columns using sand that was inoculated with induced culture (OD600 = 2.43) and flow rate (2 mL/min) gave the maximum recovery (99%) of Cr(VI). The experimental Cr(III) was successfully recycled in the tanning process and the experimental leathers showed comparable properties as same as the leathers tanned with commercial Cr(III). Thus, we concluded that using combined chemical–biological treatment system for Cr remediation from tanning wastewater together with recycling process for the recovered Cr(III) is a promising strategy for economic and environmental friendly tanning industry.

- **Keywords:** Actinomycetes; Cr(VI); Cr(III); Kitasatosporia; Microcosm; Reuse

S.S. Kalaivani, A. Muthukrishnaraj, S. Sivanesan, L. Ravikumar. *Novel hyperbranched polyurethane resins for the removal of heavy metal ions from aqueous solution*. Pages 11-23.

Novel polyurethane (PU) resin was studied for removal of Pb(II) and Ni(II) ions from aqueous solution. The resin was characterized by FT-IR, 1H NMR, 13C NMR, TGA, SEM, EDAX and DLS analysis. The optimization of experimental conditions and parameters including pH, adsorbent dosage, contact time, and initial metal ion concentration for the removal of heavy metal ion was evaluated. Batch adsorption kinetic studies were

mathematically described, and it has been found that the adsorption of Pb(II) and Ni(II) ions onto the PU follow the pseudo-second order kinetic model. Adsorption isotherms have also been studied, and the data fitted well in the order of the Freundlich > Temkin > Sips > Langmuir isotherm models. The maximum adsorption capacities of PU for Pb(II) and Ni(II) ions were calculated from the Langmuir isotherm, 236.5 and 217.5 mg/g respectively. Thermodynamic parameters such as, ΔH° and ΔG° suggest that the adsorption of Pb(II) and Ni(II) ions onto PU is exothermic and spontaneous in nature. The adsorption efficiency of the PU was retained even after five cycles. The PU has good adsorption efficiency for the removal of Pb(II) and Ni(II) ions compared to other adsorbents.

- **Keywords:** Polyurethane (PU); Adsorption; Isotherm; Kinetic; Thermodynamics; Heavy metal ions

Tomasz Janus, Bogumil Ulanicki. *Integrated benchmark simulation model of an immersed membrane bioreactor*. Pages 24-37.

This paper presents a new integrated model of an immersed membrane bioreactor (iMBR) for wastewater treatment. The model is constructed out of three previously published submodels describing the bioreactor, the membrane, and the interface between them. The bioreactor submodel extends a conventional activated sludge model with soluble and bound biopolymers which have been found to cause irreversible and reversible fouling. The membrane model describes fouling as a function of biopolymer concentrations, permeate flow, and shear stresses on the membrane surface. The interface describes the dependency of oxygen transfer rate on suspended solids concentrations and calculates shear stresses on the membrane surface from air-scour rates. The paper serves three purposes. First, the integrated model is simulated on a plant layout of a previously published MBR benchmark model which did not consider any interactions between the submodels. Hence, this paper presents a new and upgraded MBR benchmark model. Secondly, the simulation results showcase how simulations with an integrated model can be used to optimise plant performance and minimise energy consumption. Finally, the paper introduces new measures of fouling which can be used for benchmarking different MBR plant layouts and control strategies.

- **Keywords:** Benchmark model; Biopolymers; EPS; Fouling; MBR; SMP

Mehdi Amouei Torkmahalleh, Galiya Magazova, Aliya Magazova, Seyed Jamal Hassani Rad. *Simulation of environmental impact of an existing natural gas dehydration plant using a combination of thermodynamic models*. Pages 38-47.

A new approach was presented to improve the simulation results of an existing TEG based natural gas dehydration plant, using Aspen Plus software. Furthermore, the environmental impact of the plant was investigated. The plant consists of four main unit operations including an absorber, a flash tank, a stripper and a regenerator. Twelve thermodynamic models were assigned to these units. In the first step of the study, only one thermodynamic model was assigned to all of the units while in other steps, combinations of thermodynamic models were employed. The most accurate model combination was found to be RKSMHV2 for the absorber and stripper and PSRK for the flash tank and regenerator. It was found that a proper combination of thermodynamic models may improve the simulation results. As solvent circulation rate increased, BTEX, VOC and greenhouse gas emissions enhanced.

- **Keywords:** Natural gas dehydration; BTEX; VOC; Greenhouse gas; Aspen Plus; Thermodynamic models

Loi Hoang Huy Phuoc Pham, Risza Rusli. *A review of experimental and modelling methods for accidental release behaviour of high-pressurised CO2 pipelines at atmospheric environment*. Pages 48-84.

The aim of this article is to review past progress on experimental and modelling developments for depressurisation, release and dispersion of CO2 from high-pressurised pipelines. For the experimental work, several data were analysed from big projects (COOLTRANS, CO2PipeHaz, CO2PIPETRANS and COSHER) to understand release behaviours of high-pressure CO2 and to validate models developed for assessment of safety distances of CO2 pipelines. For the modelling development, mathematical and numerical models were applied to predict the thermo- and fluid-dynamical behaviours of CO2 in a broken pipeline and in a near field, and the dispersing cloud of CO2 in a far field. It was found that homogeneous relaxation model has given better predictions of the CO2 depressurisation and release than homogeneous equilibrium model. It was also found that Peng–Robinson and three-phase accurate equations of state could accurately predict the thermodynamic behaviours of CO2 in the broken pipeline and in the near field respectively. The Lagrangian particle-tracking method was found to accurately predict the far-field CO2 concentration with the presence of complex terrain. No impacts of toxic impurities (H2S, SO2) on depressurisation, release and dispersion of CO2 mixture was experimentally investigated. Further modification and validation of the novel method proposed for the high-pressure CO2 release from buried pipelines are required to accurately predict the unbalanced flow and the behaviour of solid CO2 in and around the crater. Finally, further laboratory- and large-scale experimental data are required to investigate and support validation of models predicting the impact of the toxic impurities on the CO2-mixture release.

- **Keywords:** CO2 safety; Accidental release; Phase behaviour; Experimental method; Dispersion modelling; Pressurised CO2 pipeline

Risha Mal, Rajendra Prasad, Virendra K. Vijay. *Multi-functionality clean biomass cookstove for off-grid areas*. Pages 85-94.

The burning of biomass in a traditional cookstove has led to significant particulate emissions and does not utilize the biomass efficiently. A forced draft biomass cookstove can reduce polluting emissions as compared to a traditional cookstove that is being used in developing countries. But, to achieve a cleaner combustion, it is necessary for the household to be connected with an electric supply to run the small dc-fan of such forced draft cookstoves. Thus, a thermoelectric generator (TEG) in conjunction with a biomass cookstove has been developed and deployed for electricity generation. The TEG technology deployed in a cookstove helps to run a small dc-fan even in off-grid areas. Two novel electrical circuit topologies with a TEG are presented here for the efficient power generation and clean cooking. Different types of commercially available thermoelectric generators were tested during the design & development process to obtain the required output. In addition to clean cooking, other functions such as lighting and battery charging (or mobile phone battery charging) are also available according to the user's interest and price sensitivity.

- **Keywords:** Renewable energy; Thermoelectric generator; DC–DC converter; Off-grid areas; Biomass TEG cookstove; In-door air pollution

R. Bubbico, F. Carbone, J.G. Ramírez-Camacho, E. Pastor, J. Casal. *Conditional probabilities of post-release events for hazardous materials pipelines*. Pages 95-110.

Pipelines are commonly considered a safe alternative for the transportation of hazardous materials. However, in case of failure, pipelines still pose major risks to the environment

and to the population potentially exposed. The aim of the present work is to provide occurrence probabilities of the intermediate and final events following the accidental release of hazardous materials from pipelines. A collection of incidents and accidents occurred worldwide in connection with the use of onshore long-distance pipeline networks, has been gathered to make up a specific database for the analysis of incidents in pipelines. A qualitative and quantitative analysis of the data has allowed to develop detailed event trees for the different classes of hazardous materials, and to calculate the probability of occurrence of the final outcomes. The investigation has also aimed at identifying, for each type of release, the relationship between the final events and the causes of the pipeline failure. The results obtained represent a useful and needed starting point in Quantitative Risk Analysis of hazardous materials transportation via pipelines.

- **Keywords:** Pipelines; Transportation; Accidental release; Event trees; Probabilities; Hazardous materials

Malikeh Heidari, Hamid-Reza Kariminia, Jalal Shayegan. *Effect of culture age and initial inoculum size on lipid accumulation and productivity in a hybrid cultivation system of Chlorella vulgaris*. Pages 111-122.

Chlorella vulgaris was cultivated in a hybrid (two-stage) system. The effect of the transferring time from nutrient-replete phase with a low light intensity (photobioreactor) to the nutrient deprivation phase (open pond) with a higher light intensity, as well as the effect of initial cell concentration in the deprivation phase, on the growth rate and lipid content of the microalgae was investigated. The microalgae were transferred to the nutrient deprived medium at different intervals with various initial cell concentrations. Transferring the cultivated medium of the 4th day with the initial cell concentration of 66 mg L−1 into the deprivation phase resulted in a highest lipid productivity of 9.21 ± 0.64 mg L−1 d−1 and lipid content of 53.97 ± 4.30%. In a single-stage cultivation where a medium with nitrogen deficiency was used, despite a low lipid content (maximum 30%), a lipid productivity of 9.95 ± 0.46 mg L−1 d−1 was observed that was slightly higher than that for the hybrid system.

- **Keywords:** Microalgae; Chlorella vulgaris; Hybrid system; Nutrient deprivation; Lipid productivity; Biodiesel feedstock

Gabriele Landucci, Nicola Paltrinieri. *A methodology for frequency tailorization dedicated to the Oil & Gas sector*. Pages 123-141.

The likelihood of leaks from process equipment is a key input to any Quantitative Risk Assessment. This study is aimed at developing a methodology supporting the tailorization of leak frequency values. Specific modification factors for the facilities of the Oil & Gas (O&G) upstream sector are used for this purpose. The method (TEC2O—frequency modification methodology based on TEChnical Operational and Organizational factors) is based on an aggregated set of indicators, whose contribution to the expected leak frequency is systematically evaluated through a specific procedure. Periodic revision and update represents an added value to the method, because it may be adopted to drive the identification of critical safety issues in a facility, integrating technical and managerial aspects and supporting continuous monitoring. The method is compared with similar literature methods and applied to a representative case study in order to demonstrate its potential and advantages.

- **Keywords:** Frequency modification factors; Oil & Gas; Organizational aspects; Operational aspects; Integrated operations; Quantitative Risk Assessment

Wenqing Lu, Wei Liang, Laibin Zhang, Wei Liu. *A novel noise reduction method applied in negative pressure wave for pipeline leakage localization*. Pages 142-149.

Noise in pipeline pressure signal is a small noise of which the amplitude is much smaller than that of signal. But it affects recognition of pressure drop and results in inaccurate leakage localization or false alarm. Thus, a small noise reduction method based on empirical mode decomposition (SNR-EMD) is proposed to reduce the noise in pipeline pressure signal. SNR-EMD removes the noise considered as small fluctuations in signal around the mean line calculated by signal's upper envelope and lower envelope. Meanwhile, end effect of SNR-EMD is restrained by extrema mirror extension (EME). Then tested by pressure signal in field, SNR-EMD can reduce small noise well through making the denoised signal smooth and conserving the mutation characteristics of the original signal. Finally, negative pressure wave (NPW) combined with SNR-EMD is used to locate pipeline leakage. The case study indicates that pressure drop can be well recognized and leakage can be accurately located.

- **Keywords:** Noise reduction; Empirical mode decomposition; Extrema mirror extension; Pipeline leakage; Negative pressure wave; Leakage localization

Nader Biglarijoo, Seyed Ahmad Mirbagheri, Majid Ehteshami, Simin Moavenzadeh Ghaznavi. *Optimization of Fenton process using response surface methodology and analytic hierarchy process for landfill leachate treatment*. Pages 150-160.

Typically, to treat landfill leachate, biological techniques alone are not sufficient. In this study, Fenton process was found to be effective as a pretreatment method. Analytic hierarchy process (AHP) was used to select the favorable catalyst between FeSO4 and FeCl2 when three criteria, namely, (i) COD removal, (ii) sludge to iron ratio, and (iii) risk were considered. Meanwhile, response surface methodology was applied to model and optimize three target responses, (i) COD removal, (ii) sludge to iron ratio, and (iii) organic removal to sludge ratio. The effective variables included pH, [H2O2]/[Fe2+], Fe2+ dosage and reaction time. In addition, to minimize the danger, generated sludge was reused in the Fenton process. According to AHP sensitivity analysis results, priority percentage for FeCl2 and FeSO4 were 64% and 36%, respectively. Additionally, according to the statistical analysis, all suggested models were adequate (with R2 of 0.9171–0.9617). The optimum condition was found to be pH = 6, [H2O2]/[Fe2+] = 20 mole ratio, [Fe2+] = 170 mM, and reaction time = 105 min. Results showed that [H2O2]/[Fe2+] and [Fe2+] are significant for COD removal while pH and [H2O2]/[Fe2+] were important factors for sludge to iron ratio (SIR) and organic removal to sludge ratio (ORSR), respectively. Meanwhile, when iron sludge was reused as catalyst, the results were acceptable even after five times regeneration.

- **Keywords:** Leachate treatment; Fenton process; Response surface methodology; Analytic hierarchy process; Iron sludge reuse; Advance oxidation

Weng Hui Liew, Mimi H. Hassim, Denny K.S. Ng. *Systematic framework for sustainability assessment on chemical production pathway: Basic engineering stage*. Pages 161-177.

Assessment on sustainability of production pathway is an important step to promote the sustainability features during early process design. The early process design can be divided into three stages, which are research and development (R&D), preliminary engineering and basic engineering. Note that, the assessment frameworks for R&D and preliminary engineering stages have been presented in our previous works. As continuation, a systematic framework for the assessment of chemical production pathway

in basic engineering design stage is presented in this work (Liew et al., 2014b, 2015). This framework emphasises on the inherent safety, health and environment (SHE) and economic performance (EP) assessment of chemical production pathway, with the integration of fuzzy optimisation approach as the multi-objective analysis tool. Following the proposed assessment framework, selection of pipe size and types of fittings is considered in this framework for improvement of inherent SHE and EP, as those selection criteria are the key design parameters at this design stage. To illustrate the application of the proposed framework, a case study on biodiesel production pathway assessment is presented.

- **Keywords:** Assessment framework; Process design; Sustainability; Inherent safety; Health and environment (SHE); Economic performance (EP)

Fabio Formisano, Antonino Fiorentino, Luigi Rizzo, Maurizio Carotenuto, Luca Pucci, Maurizio Giugni, Giusy Lofrano. *Inactivation of Escherichia coli and Enterococci in urban wastewater by sunlight/PAA and sunlight/H2O2 processes*. Pages 178-184.

Two solar driven Advanced Oxidation Processes (AOPs), namely sunlight/H2O2 and sunlight/peracetic acid (PAA), were investigated for the inactivation of two bacterial families (Escherichia coli and Enterococci) in real urban wastewater. Preliminary lab scale experiments were performed by using a solar simulator in order to evaluate the proper initial dose of H2O2 and PAA, respectively. According to the results achieved, 50 and 100 mg L−1 of H2O2 and 4 and 8 mg L−1 of PAA were chosen for the subsequent pilot scale experiments in a Compound Parabolic Collector (CPC) based reactor. The sunlight/PAA process resulted in a higher inactivation rate (3.52 log units of E. coli and 4.50 log units of Enterococci with an initial dose of 8 mg PAA L−1) compared to sunlight/H2O2 process (3.13 log units of E. coli and 2.45 log units of Enterococci with an initial dose of 100 mg H2O2 L−1) after 120 min of solar irradiation (7.42 kJ L−1 cumulative energy per unit of volume). It is noteworthy that significantly lower initial doses of PAA allowed to achieve a higher inactivation rate compared to H2O2, which makes sunlight/PAA an attractive option for wastewater disinfection in small communities.

- **Keywords:** Advanced Oxidation Processes; Compound Parabolic Collector (CPC); Hydrogen peroxide; Peracetic acid (PAA); Solar-driven processes; Wastewater disinfection

Neeraj Gerard, Raghunandan Santhana Krishnan, Senthil Kumar Ponnusamy, Hubert Cabana, Vinoth Kumar Vaidyanathan. *Adsorptive potential of dispersible chitosan coated iron-oxide nanocomposites toward the elimination of arsenic from aqueous solution*. Pages 185-195.

The present study investigates elimination of the arsenic [As(III)] spiked in water via adsorption using chitosan coated iron-oxide nanocomposites (CINs) as a robust adsorbent. The synthesized adsorbent exploits the magnetic nature of iron oxide for the separation of saturated CINs from the aqueous solution upon completion of treatment process. The optimum conditions for adsorption of As (III) using CINs were found to be pH 6.0, adsorbent dosage of 2.0 g/L and contact time of 30 min. The maximum monolayer adsorption capacity (qm) calculated using Langmuir model was found to be 267.2 mg of As(III) per gram of CINs. The separation factor (RL) was found to lie within 0–1, predicting that the adsorption of As(III) onto CINs is a reversible process. Based on the calculated heterogeneity parameter from Freundlich isotherm (n = 2.236), the process is highly favorable physisorption while the kinetics of the process was best explained by pseudo-second order rate equation. The regeneration of the saturated CINs could be performed using a simple acid–base treatment using 0.1 N HCl and NaOH. Upon

recycling the adsorbent for 5 batches of repeated adsorption studies, only a meagre 13% loss over its initial adsorption capacity was observed.

- **Keywords:** Adsorption; Arsenic; Chitosan; Magnetic; Nanocomposite; Regeneration

Jianhua Zhang, Adrian Knight, Mikel Duke, Kathy Northcott, Michael Packer, Peter J. Scales, Stephen R. Gray. *A new integrated potable reuse process for a small remote community in Antarctica*. Pages 196-208.

To meet water reuse and discharge requirements in Davis Station, Antarctica, an advanced water treatment plant (AWTP) had been designed and tested for nine months. The key design factors for operating in small communities in remote areas included low maintenance requirement (low chemical inventory, minimal onsite labour), high LRVs for pathogens, robust operation, and high automation. Based on these requirements, the seven-barrier AWTP included ozonation, ceramic microfiltration, biological activated carbon, reverse osmosis, ultraviolet radiation, calcite filtration and chlorination. The nine month test demonstrated that the plant was able to provide minimum LRVs of 12.5 for virus and bacteria, and 10 for protozoa. The overall estimated chemical consumption was lower than equivalent continuous operations elsewhere due to a reduced number of Clean in Place (CIP) cycles as compared to industry. This was achieved by optimised integration of the barriers. Furthermore, there was no functional failure of major barriers and the automated online pressure decay test (PDT) validations for MF and RO were successful. Although some minor improvements, such as a reduced frequency of RO pre-filter cartridge replacement, are still needed, the new integrated plant has fulfilled the requirements of high pathogen LRVs, remote online control and validation, and relatively low chemical consumption.

- **Keywords:** Water treatment; Environmental protection; Water reuse; Potable reuse; Advanced water treatment plant; Small community

Claudio Cameselle, Alberto Pena. *Enhanced electromigration and electro-osmosis for the remediation of an agricultural soil contaminated with multiple heavy metals*. Pages 209-217.

The remediation of agricultural soil contaminated with Cd, Co, Cr, Cu, Pb, and Zn was carried out by enhanced electrokinetic remediation using sulfuric acid or organic acids (EDTA, Citric acid and Acetic acid) as the processing fluid. The unenhanced electrokinetic treatment with DI water in the anolyte and catholyte resulted in some mobilization of the heavy metals, but only minor removal was observed. The use of EDTA and acetic acid in the catholyte favored the mobilization of the metals and the formation of chelates and complex ions. Citric acid was very effective in the solubilization and removal of heavy metals because of: (a) the acidification of the soil specimen and subsequent mobilization of metals, and (b) the enhanced electro-osmotic flow that favored the transportation of mobilized cations towards the cathode. The removal of Cd, Co, Cu and Zn was over 70%, whereas Cr and Pb showed very limited removal (below 12%) because of their strong immobilization in the soil.

- **Keywords:** Heavy metal; Agricultural soil; Electrokinetic remediation; Citric acid; EDTA; Acetic acid

Jun Deng, Jingyu Zhao, Yanni Zhang, Anchi Huang, Xiangrong Liu, Xiaowei Zhai, Caiping Wang. *Thermal analysis of spontaneous combustion behavior of partially oxidized coal*. Pages 218-224.

Research on partially oxidized coal helps in the early detection of spontaneous combustion due to secondary oxidation of the coal remaining in mined-out areas. Three types of coal samples were used in this study. A self-designed temperature-programmable experimental system was developed to investigate the spontaneous combustion characteristics of partially oxidized coal. In addition, the differences between the oxidation characteristics of a fresh and a partially oxidized coal sample were studied. The CO concentration and its production rate, the oxygen consumption rate and the heat release rate were used as macro-characteristic parameters to show the oxidation characteristics. The results show that the characteristic parameters increased faster with temperature for partially oxidized coal compared to a fresh sample up to a temperature of 110–140 °C. Above this temperature the opposite is observed.

- **Keywords:** Spontaneous combustion; Partially oxidized coal; CO concentration and production rate; Oxygen consumption rate; Heat release rate; Macro-characteristic parameters

H. Nouri, N. Zouzou, L. Dascalescu, Y. Zebboudj. *Investigation of relative humidity effect on the particles velocity and collection efficiency of laboratory scale electrostatic precipitator*. Pages 225-232.

This paper presents the results of an experimental investigation of corona discharge in Wire-to-Plane Electrostatic Precipitator (WP-ESP). The influence of relative humidity level (RH) on the collection efficiency of a WP-ESP is analyzed. Experimental investigations of the humidity effect on corona discharge in electrostatic precipitator are of interest for the interpretation of electrical conduction and collection efficiency phenomena in high electric fields. The experiments were performed with incense smoke particles having a mean size of about 0.28 μm. An aerosol spectrometer was employed for characterizing the size distribution of these particles at the outlet of the ESP. Then, the collection efficiencies were measured for relative humidity levels of 40 and 70%. Various DC applied voltages in the case of positive and negative polarities have been under consideration. For given atmospheric conditions, the results obtained with the aerosol spectrometer show that the performance of the ESP increases with the applied voltage (range: 10–40 kV). Also, the collection efficiency is higher at increased RH. The negative corona discharge is overall more effective than the positive one. However, the difference between the two polarities becomes minor at high RH. The performances of the ESP are improved at elevated humidity probably due to the enhancement of the particle charging in the inter-electrode gap on one hand, and the particle cohesivity on the collecting electrodes on the other hand.

- **Keywords:** Electrostatic precipitators; Corona discharge; Relative humidity; Sub-micrometer particles; Migration velocity; Collection efficiency

Jayna Pessuto, Bianca Santinon Scopel, Daniele Perondi, Marcelo Godinho, Aline Dettmer. *Enhancement of biogas and methane production by anaerobic digestion of swine manure with addition of microorganisms isolated from sewage sludge*. Pages 233-239.

In this paper, biogas was produced by anaerobic digestion (AD) of swine manure. This study aimed to isolate, select and identify microorganisms able to increase waste conversion into biogas rich in methane. These microorganisms were isolated from sewage sludge after the beginning of the AD process. Inocula of isolated microorganisms were added to the samples of swine manure. The animals from which the manure was obtained were fed with oat (O) or with swine feed (F). Inoculum addition increased methane mole fraction for O-manure sample from 0.35 to 0.60 and for F-manure sample from 0.40 to 0.70 (average values). An experimental design (2k) was used to determine statistical significance of liquid medium addition and initial pH value. Both factors had a

significant effect on the methane volume produced. In summary, microorganisms addition increased biogas volume and the methane mole fraction in it.

- **Keywords:** Anaerobic digestion; Swine manure; Inoculum; Biogas; Isolation; Methane

Weimin Cheng, Haiming Yu, Gang Zhou, Wen Nie. *The diffusion and pollution mechanisms of airborne dusts in fully-mechanized excavation face at mesoscopic scale based on CFD-DEM*. Pages 240-253.

In order to explore the diffusion and pollution mechanisms of high-concentration dusts produced in the fully-mechanized excavation face towards the operation area in the tunnel at mesoscopic scale, this article investigated the diffusion behaviors of dust particles based on CFD-DEM coupling model and field measurement. The results show that the wind vortex fields, specifically, two large horizontal vortex fields (2–10 m and 10–25 m away from the heading face) and a large vertical vortex field (0–5 m away from the heading face). For dust particles of various sizes, the diffusion distance exhibited a linearly increasing trend versus time while the maximum diffusion velocity followed a logarithmically decreasing trend with respect to the diffusion distance, the ratio of trajectory deviation of the dust particle exhibited an nonlinearly increasing trend versus dust particles sizes. The settlement of dust particles mainly occurred in two regions, which were 0–8 m and 25–35 m from the heading face. Moreover, larger dust particles settled more easily, with the settling rate up to 84.5%, while fewer respirable dusts settled, only approximately 46.7%. The dust prevention should be adopted by considering the specific diffusion distance and pollution mechanisms of the dust particles with different sizes.

- **Keywords:** Fully-mechanized excavation face; Airborne dust; Diffusion mechanism; CFD-DEM; Single-pressure ventilation; Occupational health

Saeed Eini, Hamid Reza Shahhosseini, Majid Javidi, Mahdi Sharifzadeh, Davood Rashtchian. *Inherently safe and economically optimal design using multi-objective optimization: The case of a refrigeration cycle*. Pages 254-267.

The economic viability of industrial processes strongly depends on their safe and reliable operation. The method of inherent safe process design enables systematic consideration of safety measures in order to ensure process safe operation at the early stages of process design. The challenge is that the economic measures that are often considered for the design of industrial processes are often incommensurable with the safety measures. In the present research, a novel framework is proposed in which the safety criteria are quantified based on consequence modeling and aggregated with the economic performance using multi-objective optimization programming. The developed methodology was applied to the design of a simple refrigeration cycle. The optimization algorithm was NSGA-II. The results suggested a strong trade-off between the competing economic and safety objectives in terms of Pareto frontiers that clearly quantified the required compromise. It was observed that only with a minor increase in the capital investment, it is possible to significantly improve the safety. While the case of the refrigeration cycle was selected as a demonstrating case, the research methodology is to large extend general and deemed to be acceptable to design and operation of other industrial processes.

- **Keywords:** Inherent safety; Consequence modeling; Multi-objective optimization; Layout optimization; Simple refrigeration cycle; Pareto front

Zhilin Xi, Ang Li. *Characteristics of thermoplastic powder in an aqueous foam carrier for inhibiting spontaneous coal combustion*. Pages 268-276.

For retarding self-heating of coal, a technique is described by applying a blend of thermoplastic and coal powder (TCP) in a foam carrier. The experimental study includes the behavior, microstructure and evolution of the foam, and the properties of the thermoplastic powder (TP) for inhibiting the spontaneous combustion of coal. It was found that increased TCP concentrations led to decreased foamability, with the detrimental effect on foamability levelling of at concentrations above 30 wt.%. The low fusing temperature and high heat of fusion of the TP absorbed the heat generated by the self-heating coal at low temperatures. The liquid fused TP sealed gaps and cracks in the coal dust from oxygen entry. Infrared spectra showed that the TP suppressed alkyl and hydroxyl functional groups in the coal powder (CP) at higher temperatures. It was concluded that TP retarded self-heating in coal, and that the combined thermoplastic and coal powder in a foam carrier has the potential to prevent and control the spontaneous combustion of coal.

- **Keywords:** Aqueous foam; Coal powder; Self-heating of coal; Flame retardant; Thermoplastic powder

Juliane Fiates, Sávio S.V. Vianna. *Numerical modelling of gas dispersion using OpenFOAM*. Pages 277-293.

In the current work the rhoReactingBuoyantFoam solver was customised for performing gas leak and gas dispersion modelling. Using experimental data from gas leaks the proposed modelling was investigated for subsonic and sonic releases. The gas molar fraction and velocity decay along the jet centreline were calculated using the modified reacting solver, and the numerical findings were compared with available experimental data. Different approaches for the turbulence closure problem were considered using standard two-equation models. The numerical stability of the solver was also investigated varying the CFL number for a set of simulations. The work also considered the modelling of gas cloud volume in a real engineering case. Standard computational setup for ANSYS-CFX was applied, and the same set of scenarios were modelled in OpenFOAM using the modified rhoReactingBuoyantFoam solver. The analysis considered 5 different leak directions and 4 wind directions in a typical industrial site. For all scenarios simulated, very good agreement with experimental data and with the commercial CFD (computational fluid dynamics) tool considered in this study was observed. The results are within 10% tolerance intervals. Detailed information of the modelling is also provided, which enable any CFD user to reproduce the results and also apply it for future analysis.

- **Keywords:** Computational fluid dynamics (CFD); Jets; Gas dispersion; OpenFOAM; ANSYS-CFX; Open source code; Consequence modelling

J. Lladó, Montserrat Solé-Sardans, Conxita Lao-Luque, E. Fuente, B. Ruiz. *Removal of pharmaceutical industry pollutants by coal-based activated carbons*. Pages 294-303.

Several studies have demonstrated the presence of pollutants from the pharmaceutical industry in surface and groundwater. The main inputs of pollutants come from households, hospitals and the industry and many of these compounds are not completely removed by WWTPs. The purpose of this research is to study the adsorption of paracetamol, phenol and salicylic acid using coal-based activated carbons. A lignite from Mequinenza (M) and an anthracite from Coto Minero Narcea (CN) from Spain were chemically activated with alkaline agents obtaining two activated carbons (MAC and CNAC). Two commercial activated carbons widely used in water treatment (F400 and NPK) were selected for comparison purposes. The activated carbons were characterized

and the results showed a high surface BET (1839 m2 g−1) and total pore volume (0.83 cm3 g−1) on CNAC while MAC was characterized by high sulphur content (6%). Vapour isotherms indicated a chemical interaction between the surface functional groups of MAC and the water molecules. The highest uptake of the three pharmaceutical compounds was achieved by CNAC. MAC showed a high affinity for anion salicylates (at pH 4–8). The maximum adsorption capacity of the pollutants onto the activated carbons followed the order salicylic acid > phenol > paracetamol which can be explained by hydrophobicity.

- **Keywords:** Pharmaceutical-pollutants; Modelling-adsorption; Activated-carbon; Lignite; Anthracite

Akiko Segawa, Satoshi Yoshikawa, Takayuki Toyama, Hayao Nakanishi, Emi Kikuchi-Uehara, Masahiko Hirao, Hirokazu Sugiyama. *Method for reducing environmental, health, and safety risks in active pharmaceutical ingredient manufacturing based on multiobjective evaluation*. Pages 304-313.

This work presents a method for assessing and retrofitting the manufacturing processes of active pharmaceutical ingredients (API) considering the risks caused by the environment, health, and safety (EHS), as well as economic and technical aspects. This method consists of four steps: (1) process mass analysis, (2) EHS risk evaluation, (3) generation of improvement options, and (4) multiobjective evaluation and interpretation. A new indicator is proposed as a base for risk evaluation, which considers the dynamic change in process risks as well as the technical countermeasures in the process. The multiobjective evaluation supports the identification of promising improvement options regarding the risk-reducing potential of EHS, economic performance, and the efforts of change management according to Good Manufacturing Practice. A case study was performed in an industrial API manufacturing plant, which includes charging, reaction, filtration, extraction, crystallization, centrifugation, crystal-form conversion, crystallization, filtration, and drying. By following the method step by step, a promising option could be identified that could effectively reduce EHS risks with reasonable efforts in the economic and regulatory aspects.

- **Keywords:** Pharmaceutical manufacturing; Process retrofitting; Hazard; Risk; Good Manufacturing Practice; Expert knowledge

Thi-Huong Pham, Byeong-Kyu Lee, Jitae Kim. *Improved adsorption properties of a nano zeolite adsorbent toward toxic nitrophenols*. Pages 314-322.

In this study, synthesized nano zeolite (NZ) was applied for the removal of 3 nitrophenol isomers (meta, ortho and para) to evaluate its feasibility as an effective adsorbent. NZ was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), inductively coupled plasma optical emission spectroscopy (ICP-OES) and gas adsorption analysis (BET) methods to determine its basic physicochemical properties. Adsorption experiments were carried out as a function of pH, contact time, adsorbent dose and initial nitrophenols concentration. NZ with greatly improved surface area was particularly effective for the removal of nitrophenols. The adsorption of nitrophenols onto NZ reached equilibrium within 150 min. The maximum adsorption capacities of NZ for meta, ortho and para-nitrophenols were 125.7, 143.8 and 156.7 mg/g, respectively. The adsorption behavior of nitrophenols was fitted better by the Freundlich isotherm than by the Langmuir isotherm. The regeneration characteristics of nitrophenol-loaded NZ were analyzed. Even after 5 cycles of adsorption-desorption, the percentage removal of o-, m- and p-nitrophenols were maintained at more than 70% of the initial values. The required adsorption cost for treating 1000 kg wastewater containing 300 mg/L of nitrophenols by

using NZ was 46.6% lower than that by activated carbon (AC). Based on these findings, NZ, with its low adsorption cost and high adsorption capacity, can be utilized as a more economic and effective adsorbent for nitrophenols removal.

- **Keywords:** Nano zeolite; Economic effect; Nitrophenols; Adsorbent; Regeneration; Adsorption cost; Wastewater

Pei San Kong, Mohamed Kheireddine Aroua, Wan Mohd Ashri Wan Daud, Patrick Cognet, Yolande Pérès. *Enhanced microwave catalytic-esterification of industrial grade glycerol over Brønsted-based methane sulfonic acid in production of biolubricant*. Pages 323-333.

The industrial production of renewable lubricant glycerol trioleate was simulated using a microwave reactor through esterification of glycerol with oleic acid in the presence of methane sulfonic acid catalyst under solvent-free conditions. The interaction effects of operating temperature, catalyst concentration, and reaction time were investigated. A conversion of 90% was achieved in optimal conditions (191 °C, 0.3 wt% and 104 min reaction time) and reduced pressure environment. This result was impressive, compared to the conversion abounded with conventional reactor (39.5%). Furthermore, two different industrial grade crude glycerols were used as starting materials to evaluate the effect of impurities. The findings confirmed that the presence of impurities reduced both selectivity and total conversion significantly.

- **Keywords:** Esterification; Glycerol; Methane sulfonic acid; Microwave; Conventional; Impurities

Mohammad Malakootian, Maliheh Pourshaban-Mazandarani, Hiwa Hossaini, Mohammad Hassan Ehrampoush. *Preparation and characterization of TiO2 incorporated 13X molecular sieves for photocatalytic removal of acetaminophen from aqueous solutions*. Pages 334-345.

Although stabilizing of nano-particles on porous media is a suitable methods in harnessing the agglomeration and inactivation of nano-particles, but still release of particles to the environment remains the most serious challenges facing toward photocatalysis process. Attachment of nanoparticles through ion exchange may be a promising method to solving these defects. In this study TiO2 was incorporated into the 13X molecular sieves by addition of the titanyl ion through an ion-exchange of ammonium-titanyl-oxalate as well as the decomposition of titanyl oxalate salt, which remained on the zeolite through the impregnation and calcination process. A part of TiO2 on the zeolite was also bound through a TiOSi bond. The investigation of TiO2-HX catalytic potential showed that neutral pH and 500 mg/L catalyst were the optimal conditions for acetaminophen removal (1 mg/L) in the UV/TiO2-HX process. The maximum removal efficiency of 95.45% ± 0.8 was attained after 75 min contact time. The acetaminophen degradation during the UV/TiO2-HX process was followed a pseudo first order kinetic model with rate constants (Kapp) of 0.8676 h−1. Under the optimum conditions, maximum synergistic efficiency of 60.07% was acquired. The experimental data showed that the UV/TiO2-HX process is effective in acetaminophen removal from aqueous solutions.

- **Keywords:** NaX zeolite; Pharmaceuticals; Photocatalysis; TiO2; Ion exchange; Acetaminophen

Thillai Sivakumar Natarajan, Hari C. Bajaj, Rajesh J. Tayade. *Palmyra tuber peel derived activated carbon and anatase TiO2 nanotube based*

***nanocomposites with enhanced photocatalytic performance in rhodamine 6G dye degradation*. Pages 346-357.**

Activated carbon (AC) was synthesized from Palm tree fruit waste material (peel of Palmyra tuber), subsequently AC-loaded anatase TiO2 nanotube (ATNT) composite was synthesized by alkali hydrothermal method using anatase TiO2 nanoparticles (ATNP). The synthesized activated carbon/anatase TiO2 nanotube (AC/ATNT) composites were characterized using powder X-ray diffraction, scanning electron microscopy, transmission electron microscopy, surface area, and UV–vis diffuse reflectance spectroscopy analysis. SEM and TEM analysis revealed the tubular morphology of the ATNT and AC/ATNT composites. The enhancement in the surface area of ATNT and AC/ATNT composite materials as compared with ATNP and pristine ATNT further validated the tubular morphology of ATNT and successful synthesis of AC/ATNT composites. The photocatalytic activity evaluation results revealed that 10%-AC/ATNT composite showed enhanced photocatalytic degradation performance (85%) in rhodamine 6G (RhB-6G) degradation as compared to pristine ATNT (78%), Degussa P-25 TiO2 (P25, 60%), and ATNP (56%). The incorporation of AC efficiently enhanced the adsorption quantity of RhB-6G dye, improved the visible light response and decreased the rate of photogenerated electron–hole recombination resulting in significantly enhanced photocatalytic performance of AC/ATNT composite. RhB-6G dye degradation was further confirmed by chemical oxygen demand (COD) and total organic carbon (TOC) analysis. The result concluded that tubular morphology, synergic effect, enhanced adsorption, and efficient decrease in the photo-produced charge carrier recombination are reasons for the enhanced photocatalytic degradation performance of AC/ATNT composite material in the degradation of RhB-6G dye using our current reaction conditions.

- **Keywords:** Palmyra tuber; Activated carbon; TiO2 nanotube; AC/ATNT composite; Rhodamine 6G; Photocatalysis

John Frederick D. Tapia, Jui-Yuan Lee, Raymond E.H. Ooi, Dominic C.Y. Foo, Raymond R. Tan. *Planning and scheduling of CO2 capture, utilization and storage (CCUS) operations as a strip packing problem*. Pages 358-372.

CO2 capture, utilization and storage (CCUS) is an important carbon management strategy that involves capturing CO2 from flue gas, transporting it, utilizing it for economically productive activities (carbon capture and utilization, or CCU), and/or permanently disposing it in non-atmospheric sinks (carbon capture and storage, or CCS). Some technologies, such as enhanced oil recovery (EOR) allow simultaneous CCUS, while other alternatives are either purely CCS (e.g., geological storage) or purely CCU (e.g., use of CO2 as a process plant feedstock). In this work, CCUS is addressed in the context of a large-scale CO2 chain that contains both CCS and CCU options. It is necessary to consider the availability of CO2 sources and sinks to develop a profitable allocation plan for such CCUS systems. Thus, a modeling framework using a geometric representation is proposed to optimize both scheduling and allocation in a CCUS system, given multiple CO2 sources and sinks. Two mixed integer linear programming (MILP) models are developed to address three important factors for planning downstream CCUS operations, i.e., scheduling of CO2 capture and EOR operations, allocation of CO2 supply for EOR operations, and source–sink matching subject to injectivity and capacity constraints. Two case studies are then solved to illustrate the two MILP models.

- **Keywords:** CO2 capture; Utilization and storage (CCUS); Enhanced oil recovery (EOR); Continuous-time optimization; Mixed integer linear programming (MILP); Strip-packing problem

Xianfang Zhu, Tiehong Song, Zhuo Lv, Guodong Ji. *High-efficiency and low-cost α-Fe2O3 nanoparticles-coated volcanic rock for Cd(II) removal from wastewater*. Pages 373-381.

Volcanic rock with the α-Fe2O3 nanoparticles coating was fabricated to be an efficient and low-cost adsorbent for Cd(II) ions in water. ESEM, TEM, XPS and BET characterizations of the coated volcanic rock showed that the α-Fe2O3 nanoparticles were successfully and homogeneously disseminated throughout the rock, including penetration into rock pores. Batch experiments were conducted to examine adsorption performance. The highest adsorption values were observed in a pH range of 4.0-7.0; hence, a pH value of 6.0 was used in this study. The maximum adsorption capacities of Cd(II) ions were found to be 127.23 mg/g, 146.41 mg/g and 158.48 mg/g at 293 K, 303 K and 313 K, respectively. The adsorption kinetic features of Cd(II) ions were found to be fitted best by a pseudo-second-order model, suggesting the presence of chemisorption processes. Intra-particle diffusion model results show that the adsorption processes can be divided into different stages, and the adsorption of the exterior and interior surfaces reached saturation at approximately 40 and 240 min, respectively. The adsorption process was also found to be endothermic and spontaneous. Hence, volcanic rock coated with α-Fe2O3 nanoparticles serves as a high-efficiency and low-cost adsorbent.

- **Keywords:** α-Fe2O3 nanoparticles; Volcanic rock; Cd(II) ions; Adsorption; Adsorbent; Wastewater

Jen-Chih Yang, Pao-Erh Chang, Wei-Chu Chie, Jen-Pei Liu, Chang-Fu Wu. *Large-scale search method for locating and identifying fugitive emission sources in petrochemical processing areas*. Pages 382-394.

Background: Fugitive emission sources generated from leaking components are often difficult to identify and locate, especially in petrochemical processing areas, which have concentrated facilities and equipment. **Methods:** A large-scale search method for locating and identifying fugitive emission sources in a petrochemical processing area by using multiple intersecting open-path Fourier transform infrared (OP-FTIR) beam paths and multivariate statistical methods is proposed in this study. Multivariate statistical methods, namely principal component analysis (PCA) and correspondence analysis (CA), were applied to the measured data set and the characteristics of emission sources were summarized. **Results:** Styrene, 1,3-butadiene, cyclohexane, ammonia, ethylene, propylene and methanol were identified in most beam paths with mean concentrations up to 75.3 ± 11.4 ppbv, 355.2 ± 34.6 ppbv, 188.1 ± 17.82 ppbv, 255.57 ± 19.28 ppbv, 194.3 ± 18.2 ppbv, and 94.0 ± 16.7 ppbv, respectively. PCA extracted at least three source categories in the plant. CA provided additional information about the approximate locations of each source, and thus, future emission reduction plans can be developed accordingly. **Conclusion:** This study established a dynamic approach for locating fugitive emission sources in a complex petrochemical plant by applying an OP-FTIR matrix-path approach combined with PCA and CA. Future emission reduction plans can be developed according to the findings of PCA and CA.

- **Keywords:** Fugitive emission sources; Petrochemical plant; Open-path Fourier transform infrared (OP-FTIR) spectrometry; Matrix-path approach; Principal component analysis; Correspondence analysis

H. El Knidri, R. El Khalfaouy, A. Laajeb, A. Addaou, A. Lahsini. *Eco-friendly extraction and characterization of chitin and chitosan from the shrimp shell waste via microwave irradiation*. Pages 395-405.

For the first time, the chitosan was prepared through a fast, easy and efficient method, by using a microwave irradiation in the three steps of the extraction: demineralization,

deproteinization and deacetylation. A comparative study was performed by using the conventional heating method to prepare chitin and chitosan. The structure and physicochemical properties, especially the degree of deacetylation DD%, of the chitin and chitosan obtained by these two methods were characterized by Fourier-Transform Infrared Spectroscopy FTIR, Nuclear Magnetic Resonance spectroscopy NMR, X-ray Diffractometry XRD and Scanning Electron Microscopy SEM equipped with energy dispersion spectroscopy EDS. It was shown that chitosan, with a degree of deacetylation of 82.73%, was successfully prepared in 24 min via microwave irradiation method, while a much longer time of 6–7 h was needed for preparing chitosan with a same degree of deacetylation (DD = 81.5%), using a conventional heating method. The microwave technology has allowed a great reduction of the extraction time, about 1/16. These results revealed that microwave irradiation is a more energy saving, more efficient and environment-friendly way to valorize shrimp waste.

- **Keywords:** Chitosan; Green chemistry; Degree of deacetylation; Biomaterial; Microwave irradiation; Chitin

P. Asaithambi, Baharak Sajjadi, Abdul Raman Abdul Aziz, Wan Mohd Ashri Bin Wan Daud. *Performance evaluation of hybrid electrocoagulation process parameters for the treatment of distillery industrial effluent*. Pages 406-412.

A hybrid electrocoagulation process using iron electrode was developed for removal of organic pollutants from distillery industrial effluent. Combinations of electrocoagulation process with different advanced oxidation processes such as electrocoagulation, photo–electrocoagulation, peroxi–electrocoagulation and peroxi–photo–electrocoagulation processes investigated and compared in terms of color removal, Chemical Oxygen Demand (COD) removal and electrical energy consumption. An overall COD removal efficiency of 85% with 1.20 kWh/m3 of energy consumption, current density of 0.13 A/dm2, initial COD concentration of 2500 ppm, initial pH of 7, H2O2 concentration of 234 mg/L, stirring speed of 100 rpm and reaction time of 240 min was observed in the peroxi–electrocoagulation process. The effects of different operating parameters such as initial pH of the effluent (3–11), current density (0.03–0.23 A/dm2) and concentration of H2O2 (58.5–585 mg/L) on color removal, COD removal and electrical energy consumption were studied. The direct- and alternating-current electrocoagulation processes were also studied.

- **Keywords:** Distillery effluent; Peroxi–photo–electrocoagulation; Alternating current electrocoagulation; Color removal; COD removal; Electrical energy consumption

Mehdi Ahmadi, Hasan Rahmani, Afshin Takdastan, Neemat Jaafarzadeh, Azar Mostoufi. *A novel catalytic process for degradation of bisphenol A from aqueous solutions: A synergistic effect of nano-Fe3O4@Alg-Fe on O3/H2O2*. Pages 413-421.

In this study, alginate–Fe2+/Fe3+ polymer coated Fe3O4 magnetic nanoparticles (Fe3O4@Alg-Fe MNPs) with core/shell structure were synthesized by a simple oxidation–precipitation method and used as a nanocatalyst in heterogeneous catalytic ozonation process to degrade bisphenol A (BPA). The characterization studies (X-ray diffraction, transmission electron microscope, X-ray photoelectron spectroscopy, Fourier transform infrared spectroscopy) confirmed that Fe3O4 core was coated with a layer of alginate–Fe2+/Fe3+. Elementary experiments with single processes were carried out to select the optimum values of BPA concentration, O3 flow rate, H2O2 concentration, and nano catalyst concentration as 10 ppm, 0.1 g/h, 30 mmol L−1 and 0.7 g L−1, respectively. The results showed that BPA degradation is strongly dependent on the pH, initial

concentrations of the catalyst, H2O2 and O3 dosage. The degradation of BPA could be due to the presence of three hydroxyls radical productions, including O3, H2O2 and Fe on Fe3O4@Alg-Fe MNPs. In order to determine the inherent (in principle possible) biodegradability of bisphenol A, the Zahn–Wellens test was used and results showed that COD related to bisphenole A was fully eliminating over 2–3 weeks.

- **Keywords:** Bisphenol A; Catalytic ozonation; Nanoparticle; Zahn–Wellens test

Shungang Wan, Zulin Hua, Lei Sun, Xue Bai, Lu Liang. *Biosorption of nitroimidazole antibiotics onto chemically modified porous biochar prepared by experimental design: Kinetics, thermodynamics, and equilibrium analysis*. Pages 422-435.

This investigation emphasized the optimum preparation conditions for the chemical modification of eucalyptus sawdust biochar as a potential biosorbent to promote the removal of nitroimidazoles from aqueous solutions. By ANOVA for central composite design of response surface methodology, we found the activation temperature and impregnation ratio of 85% H3PO4 to sawdust as the significant factors for maximizing the adsorption capacity of metronidazole. Optimum activation temperature, impregnation ratio, and activation time were 500 °C, 0.62, and 90 min, respectively. The Brunauer–Emmett–Teller surface area and total pore volume increased from 32.80 m2 g−1 to 882.04 m2 g−1 and 0.01829 cm3 g−1 to 0.4316 cm3 g−1 after H3PO4 activation, respectively. The removal efficiencies using biochar prepared at optimum conditions were 97.1% and 96.4% for metronidazole and dimetridazole at 20 mg L−1 concentration and 1.0 g L−1 biochar dosage within 2 h. The adsorption process was described well by pseudo-second-order model, and solute transfer was controlled by both boundary-layer and intraparticle diffusion. Thermodynamic study revealed that the adsorption process was spontaneous and exothermic. The Freundlich model presented better a fit for the adsorption equilibrium. The maximum adsorption capacities for metronidazole and dimetridazole were 167.5 and 200 mg g−1, respectively.

- **Keywords:** Biochar; Chemical activation; Optimization; Response surface methodology; Nitroimidazole; Adsorption mechanism

Jun Lu, Zhong-Ru Wang, Yu-Ling Liu, Qing Tang. *Removal of Cr ions from aqueous solution using batch electrocoagulation: Cr removal mechanism and utilization rate of in situ generated metal ions*. Pages 436-443.

The removal mechanism of batch electrocoagulation (EC) process for removing Cr ions was investigated. The influence of operation parameters on removal mechanisms was discussed. The utilization rate of in situ electro-generated Fe ions in the sludge was introduced to investigate the removal mechanism and optimize the EC process. The Fe elements' utilization rate resulting from the specific adsorption is much higher than that resulting from precipitation and co-precipitation. The initial pH determines which removal mechanism dominates the Cr removal. At neutral initial pH condition, Cr ions are mainly removed by flocs' surface complexation reaction (specific adsorption). The utilization rate of Fe ions at neutral pH condition reaches its maximum and is higher than that at other pH conditions. The influence of electrode material on EC performance was investigated on the basis of utilization rate of Fe ions. For EC with Fe/Al electrode combination, although direct dissolution of Al ion from Al electrodes will improve the Cr(VI) removal efficiency, the utilization rate of generated metal ions is much lower, when compared with EC with Fe/Fe electrode. The utilization rate of in situ electro-generated metal ions could be considered as a new index to evaluate EC performances.

- **Keywords:** Electrocoagulation; Mass transfer; Complexation reaction; Chrome; Batch reaction; Cr; Wastewater

Christof Lanzerstorfer. *Residue from the chloride bypass de-dusting of cement kilns: Reduction of the chloride content by air classification for improved utilisation*. Pages 444-450.

In many cement kiln systems a chloride bypass is required in order to avoid operational problems caused by the deposition of alkali chlorides. The dust collected from the bypass gas often has to be discharged to landfill sites because it is enriched in chloride. In this study classification of cement kiln bypass dust (CKBD) for chloride removal was investigated. Through air classification a fine fraction which was enriched in chloride, and somewhat less enriched in potassium, was separated from the bulk of the CKBD, thus reducing the concentration of these components in the coarse fraction of the material. This coarse fraction could be returned to the cement production process. The fine chloride-enriched fraction could be discharged to landfill sites or fed to a leaching process for the production of potassium chloride. The approximately 2–3 times higher chloride concentration of the feed material should improve the profitability of such a process. Other components enriched in the fine fraction were sodium, lead, cadmium and copper.

- **Keywords:** Cement kiln bypass dust; CKBD; Chloride; Air classification