# 4th International Chemical and Environmental Engineering Conference ICEEC 2013-14

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# Abstract Book


**World Academy of Research and Publication**

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# Preface

The Organizing Committee warmly welcomes our distinguished delegates and guests to the 4th International Chemical and Environmental Engineering Conference (ICEEC 2013-14) held in Kuala Lumpur, Malaysia. The aim and objectives of ICEEC 2013-14 is to provide a platform for researchers, engineers, academicians as well as industrial professionals from all over the world to present their research results and development activities in Chemical and Environmental Engineering. These conferences provide opportunities for the delegates to exchange new ideas and application experiences face to face, to establish business or research relations and to find global partners for future collaboration. We are pleased to have delegates from Poland, Bulgaria, Iran, Bangladesh, India, Philippine, Iran, Indonesia, Pakistan, Japan, UK and Korea. This conference is multi-disciplinary having different papers on Water and Wastewater Treatment, Gas Purification and Separation and Chemical and Environment Technology.

Selected papers will be published in the International Journal of Chemical and Environmental Engineering (IJCEE).International Journal of Chemical and Environmental Engineering is a scholarly open access, peer-reviewed, interdisciplinary, biannual and fully refereed journal focusing on theories, methods and applications in Chemical and Environmental Engineering. The journal reviews papers within possible minimum time of submission and publishes accepted articles on the internet immediately on receiving the final versions.The IJCEE has both its printed and electronic version http://www.warponline.org/journals.htm.

We would like to thank the key note speakers, program chairs, and organization staff for their contribution to the success of ICEEC 2013-14. We hope that all participants and other interested readers benefit scientifically from the proceedings and also find it stimulating in the process. Finally, we would like to wish you success in your scientific and technical presentations and social net working.

We hope you have a unique, rewarding and enjoyable week at ICEEC 2013-14 in Kuala Lumpur Malaysia.

With our warmest regards,
The Organizing Committees
February 14-16, 2013-14
KL Malaysia


# KHADIJA QURESHI

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Prof.Dr.Khadija Qureshi is Professor in Chemical and Environmental Engineering, Mehran University of Engineering and Technology, Jamshoro. She has extensive research and teaching background in chemical and environmental engineering. Since 18 years she is teaching and supervising the research projects on waste water treatment, reuse and recycling of waste materials and agricultural wastes, conversion of agriculture waste into adsorbents and coagulants and insulating materials. She has in her credit more than seventeen (17) publications published in international conferences and peer reviewed journals. She is key trainer in gender and mainstreaming, Women in leadership and management, Women and mentoring and Women in Higher Education. She is also editor of the International Journal of Chemical and Environmental Engineering.

## TREATMENT OF DRINKING WATER BY INDIGENOUS COAGULANT DEVELOPED FROM MANGO PIT USING MICROFILTRATION


### Abstract

Coagulants are widely used for the removal of turbidity caused by the presence of suspended solids and colloidal material. Salts of Aluminum and ferric are the most commonly used coagulants for the processing of tap and waste water treatments throughout the globe. These inorganic coagulants are not safe due to highly carcinogenic containments. From last two decade researchers are paying attention on the development of natural and biodegradable coagulants from plant residue and animal tissues. Developed organic coagulants were acknowledged for human health safety and produce lower quantity of sludge. Biodegradable coagulants have been successfully developed from seed of Cassia Angustifolia, seed of Nirmali, bean of Mesquite, Maize, Chestnut, Acron, Cactus Latifaria and leguminous species.

Pakistan produces almost 1.7279 million tons per year of Mango. Mango kernel mass average is 9 to 23% of mango on wet basis. In the research coagulant was prepared from indigenous mango kernel and passed from micro-filtration rig for the highest removal of generated flocks. Mango pits were collected, de-moisturized, fined, screened and chemically treated for the extraction of active compounds. Operating parameters as dose of developed coagulant, pH of turbid water sample, initial concentration of synthetic turbid and flow rate of the coagulant treated water through micro-filtration experimental rig were optimized. Results indicate 99.9% of decreases of turbidity causing suspended solids at 0.5ml/liter coagulant dose, sample pH 13 and 0.5 Liter per minute of controlled flow through the micro-filtration experimental rig. Coagulation activity of mango kernel was found to be 99%, highest as compare to the other organic (biodegradable) coagulant such as Moringa Oleifera (86 %), Chestnut (80 %) and Acorn (70 %). The developed coagulant was compared with existing inorganic commercial coagulant; results were similar to Alum (99%). It was observed that in extreme acidic and basic samples of turbid water the removal efficiency was increased.The process of extracting natural and biodegradable coagulant from mango pit is cost-effective and environment friendly in use due to protein content.

# Paper ID-01

## Heavy Metals Removal from Wastewater Using Agricultural Wastes as Adsorbents: A review

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**Abstract:**
The removal of heavy metals from wastewater by the adsorption process is being widely used by several researchers and activated carbon (AC) has been commonly used as an adsorbent. Although it's extensive use in the water and wastewater treatment industries, AC remains an expensive material. In recent years, conscientious effort has been made by researchers to produce a cheaper, more effective and environmental friendly AC that are equivalent to commercial available ones. Therefore, there is an urgent need that all possible sources of agro-based inexpensive adsorbents should be explored and their feasibility for the removal of heavy metals should be studied in detail. This paper presents an overview of some low-cost adsorbents based on recent publications and their utilization possibilities for the elimination of heavy metals from wastewater.

# Paper ID-02

## Baseline study of particulate matter levels in major urban centres in eastern Nigeria

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**Abstract:**
This study investigated the fine and coarse particulate load in fifteen urban centres in eastern Nigeria namely; Aba, Umuahia, Eket, Uyo, Nnewi, Onitsha, Calabar, Ogoja, Abakaliki, Afikpo, Enugu, Nsukka, Orlu ,Owerri and Port Harcourt in the dry and wet seasons from December, 2008 to September, 2009 using digital on-site readout instrument. The results showed that the cities' mean total suspended particulate matter (TSP), particulate matter with diameter less or equal to ten micrometer (PM10) and particulate matter with diameter less or equal to two and half micrometer (PM2.5) ranged between 15.28-1246.61µgm_3, 7.66-784.27 µgm_3 and 1.75-76.86 µgm_3 respectively. The corresponding annual mean values in microgram per cubic metre for the TSP, PM10 and PM2.5 were 207.87±30.49, 45.52±30.19 and 21.19± 50.03 respectively. The maximum annual mean levels of TSP, PM10 and PM2.5 were obtained in Onitsha urban while their minimum values of TSP and PM10 were recorded in Ogoja and PM2.5 in Calabar. The parameters monitored gave higher values in the dry season relative to wet season in all the investigated urban centres. Comparatively the cities had particulate matter load in the order Onitsha > Aba > PortHarcourt > Umuahia > Owerri > Eket > Abakaliki > Enugu > Nsukka >Uyo > Afikpo > Nnewi > Orlu > Calabar > Ogoja. The correlation matrix indicated that PM10 correlated with TSP and PM2.5 ($p < 0.05$) in all the cities. The city annual mean TSP values revealed that five cities; Nnewi, Calabar, Ogoja, Afikpo and Orlu (about 33 % of the cities studied) had their annual mean TSP values within the World Health Organisation(WHO) annual guideline limit of 60-90 µgm_3 for combined exposure to TSP and SO2. The PM10 annual mean levels in all cities except Calabar and Ogoja exceeded the United States annual NAAQS of 50 µgm_3 and seven cities: Eket ,Calabar, Ogoja, Afikpo, Enugu, Orlu and Nnewi (48% of the cities studied) were within the United States Environmental Protection Agency (UNEPA) recommended annual average limit of 15 µgm_3 for PM2.5 .The study concluded that having greater percentage (about 67 % forTSP, 87.7 % for PM10 and 52 % for PM2.5) of the cities studied exceeding the recommended annual guideline limit portends public health risk particularly to people dwelling in the affected cities.

# Paper ID-03

## Measuring and Modeling of $CO_2$ and $SO_2$ dispersion and emission from gas flaring:A case study of south pars gas complex second refinery,IRAN.

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**Abstract:**
Because of variation of combustion efficiency in oil and gas refineries, flaring gases may have harmful environmental and unsafe effects. Combustion of these gases in flare tip releases different hazardous products including CO2, SO2, and others suspend matters as well as simultaneous radiation result in harmful environmental and social impacts. In this study, the main aim was evaluation of amount of pollutant gases and hydrocarbons emission delivered in flare zone using different methods in different locations of South Pars Gas Complex Second Refinery,Iran. The amounts of the pollutant emission were obtained by three methods based on emission factor model, stoichiometric combustion reactions and special sampling device on the ground level as a practical way. There is a good agreement between the results and standard range of environmental protection agency data (EPA). Furthermore, the presented emission factor model is applicable for industrial complexes and reliable for pollutant emission prediction in plant scale. Distribution and dispersion of pollutants concentration has been evaluated by using Gaussian Plume model in various locations of the source. The pattern of pollutants concentration dispersion was determined for three cases of gas flow rate namely: turndown case, normal case, and design case. Comparison of the measured data with the concentrations predicted by the model shows a good agreement between them

# Paper ID-04

## Degradation of odorous compounds from food production by oxidation methods

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**Abstract:**
Odorous compounds present in off-gases emitted as a result of industrial processes constitute a considerable part of environmental pollution. Deodorization of these gases raises a crucial issue in terms of environmental engineering as well as the human comfort of living and working. The aim of the work was to examine degradation efficiency of malodorous compounds originating from the selected food industry plants under the influence of ozone and low-temperature plasma environment. The research covered two yeast processing plants and an industrial brewery. The investigated material comprised a baker's yeast broth and a brewer's wort which were taken from the proper fermentation tanks during industrial processes. In laboratory conditions the liquor was placed into a container equipped with a heater inside and a disc diffuser at the bottom. During the experiment the container content was warmed up and the air supplied by the blower was passed through the diffuser. The mixture of air and volatile compounds was directed into the reaction environment where the degradation took place. Series of experimental tests of the degradation of malodorous compounds were conducted with the use of ozone, low-temperature plasma environment and both methods simultaneously with variable process conditions. Basing on literature data and own research a plasma-chemical reactor with dielectric barrier discharges (DBD) was constructed and used. Several parameters were measured in the system, such as active power supplied to the reactor as well as temperature and humidity of the entering gas mixture. By changing volumetric rate of air flow, different residence times in the reaction zone were obtained. Samples of contaminated air before and after the reactor were taken with the use of SPME (Solid-Phase MicroExtraction) technique. Efficiency of the process was determined by evaluating the degradation rates for the identified volatile compounds. Qualitative and quantitative analysis was performed using gas chromatography / mass spectrometry system.

# Paper ID-05

## Influence of filtering layer thickness on hydrogen sulphide removal from air

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**Abstract:**
The present studies were focused on the possibility of removing small amounts of hydrogen sulphide by catalytic oxidation with atmospheric oxygen. Utilization of ferric chelates in the process is widely known. The catalyst is active in strong alkali environment which causes serious corrosivity problems. To avoid these problems fibrous ion exchangers as carriers of the catalyst were used. The role of fibrous package is improving the mass-transfer between the gas and liquid, buffering the pH of absorbing solution and catalyzing the reactions of oxidation of sulphur and iron ions. The main parameters affecting the process of catalytic oxidation are: concentration of hydrogen sulphide in the air, relative humidity of the purified air, the process time and the content of Fe-EDTA complex in the fibres. It has been established that degree of conversion of hydrogen sulphide to sulphur was 70-90% if the residence time of the purified air in the mass-exchange unit was 0.35 second. It allows to apply very thin filtering layers of the Fe-EDTA/Fiban AK-22 material as an efficient mean for hydrogen sulphide removal. The most perspective area of their application is air purification and individual protection of human from harmful impurities.

# Paper ID-06

## INDOLIBERTi Pipe Filter: An Innovation Pipeline to Decrease Water Pollution of Domestic Waste Fluid

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**Abstract:**
The high rate of population growth in Indonesia, especially in big cities increases the demand of housing for their living. These problems will cause environmental problems such as water, soil, and air pollution, also environmental degradation. The main issues that will arise and have to be anticipated is water pollution from domestic waste. Domestic waste is the largest contributor to waste on this earth example is the waste industry and market. Increase in the number of domestic waste, especially the waste fluid will cause the water to be contaminated and can not be consumed either for bathing, washing, or latrines. Whereas at this point the need for clean water is very high. Wastewater treatment technologies at this time run is less effective, because of high operational costs and complexity of the operating system. Based on these considerations necessary domestic wastewater treatment system that is more simple, practical, inexpensive, and easy to manufacture and operate. INDOLIBERTi pipe filter is a filter that innovation pipeline which has the advantage of cheap, easy, and safe for use where there is a composite zeolite and TiO2 content of polluting substances in order to minimize the domestic waste both organic and inorganic compounds through photolysis process. It will be good not only for society but also for the environment.

# Paper ID-07

## Recovery and Reuse of Platinum catalyst from used fuel cells.

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**Abstract:**
The demand for hard disks and fuel cell are increasing. Electrochemical reactions of polymer electrolyte fuel cell consist of at the anode and cathode of the oxidation-reduction reaction. Two electrodes, cathode and anode, are separated by a polymer electrolyte membrane.Oxidation and reduction reaction rate is very slow at temperatures below 100 ℃, so the use of a platinum catalyst to increase reaction rate. Cathode electrode to increase in the oxygen reduction reaction activity requires a large amount of platinum. But, depending on the cell cost increases to reduce the amount of platinum has been studied. In this study, we can recovery and reuse platinum from used fuel cell membrane assembly because lack of demand and rising prices of platinum. The electrode properties were investigated for use of an electrode catalyst.

# Paper ID-08

## Architecture of environmentally functional open spaces by two-dimensional nano assembly

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**Abstract:**
Two-dimensional nanomaterials, as e.g., inorganic layered-clay mineral, graphene, and metallic nanosheet, have been attracting increasing interest in the field of environmental sciences owing to their unique properties on catalysis, adsorption as well as electronic transportation. In the present study, open spaces formed by two-dimensional nanomaterials with the sizes ranging from angstrom to nanometer are specifically highlighted. We explore environmental functionality as, e.g. CO2 adsorption, induced by local molecular structures characteristic for two-dimensional nanomaterials.

# Paper ID-10

## Kuwait Environmental Remediation Program (KERP): Remediation Demonstration Strategy

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**Abstract:**
Kuwait had 114 square kilometers of its desert severely damaged by 798 detonated oil wells at the hands of Iraqi Troops. Crude oil gushed from the damaged oil wells, forming lakes that contaminated over 40 km2 of the land. Consequently, wet and dry oil lakes were created in low-lying areas of the desert and contaminated soil piles were generated during the recovery phase to stop the spread of oil. Contaminated land desert altered soil properties, which caused the deaths of plants (e.g. biota) and animals; and penetrated deeper into the soil layers and threatening pollution of precious groundwater resources. The United Nation Compensation Commission (UNCC), Kuwait National Focal Point (KNFP), Kuwait Institute of Scientific Research (KISR), and Kuwait Oil Company (KOC) cooperated in a joint project to undertake comprehensive efforts to remediate the approximate 26 million cubic meters of heavily oil contaminated soils. Demonstration remediation technologies are sought as viable solutions to develop suitable action plans for remediating the heavily oil contamination soil. The objective of this field demonstration study is to determine the viability, applicability and effectiveness of proven remediation technologies in treating oil contaminated soil. This project will be implemented within selected sites in the KOC's operational oil fields in South-East Kuwait (SEK) to remediate of three features (i.e. wet, dry oil lakes and oil contaminated piles). A successful remediation technologies demonstration project will be a key indicator for developing soil remediation strategy plans for full-scale implementation in SEK and other eligible areas.

# Paper ID-12

## Treatment of Water Hyacinth and Pineapple Indigenous Fibers for Textile Applications using Plasma Enhanced Chemical Vapor Deposition (PECVD)

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**Abstract:**
The effects of plasma treatment on chemical and physical properties of indigenous fibers such as water hyacinth and pineapple were investigated. Oxygen, argon, hydrogen and mixed oxygen/argon gases were used to produce plasma in a plasma-enhanced chemical vapour deposition device. Yarns were produced from the plasma treated indigenous fibers with 80% polyester, 10% water hyacinth and 10% pineapple composition. Properties of textiles made from yarns were further characterized by scanning electron microscopy fitted with energy dispersive x–ray (SEM-EDX), x-ray diffraction analysis (XRD), thermogravimetric analysis (TGA), contact angle, dyeability, air permeability, color quality thru percent reflectance, and laundering. Results show that textiles made from plasma treated indigenous fibers such as water hyacinth and pineapple possess comparable properties of commercial 100% polyester textiles.

# Paper ID-13

## Optimization of Oxidative- Adsorptive Desulfurization of Diesel Fuel Using High Shear Mixer With Chitosan-Coated Bentonite (CCB)

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### Abstract:
The increase of worldwide consumption of fuel has resulted in environmental and health hazards arising from elevated concentrations of sulfur dioxide and sulfate particulate matter in the atmosphere. To reduce the sulfur content in diesel fuel, oxidative desulfurization (ODS) was first studied. One of the important factors that affects the conversion of sulfur compound and accelerate the reaction is agitation. It is known that the reaction of sulfur compounds in fuel with an oxidant is considerably slow, therefore determining appropriate mixing techniques is important for the enhancement of the system. In this paper, oxidative desulfurization of sulfur compounds using hydrogen peroxide, phosphotungstic acid, and phase transfer agent by means of high shear mixer were described. The agitation speed (8000 – 12000 rpm), reaction temperature (60 – 80 oC), and treatment time (20 - 40 min) were chosen as parameters and optimized using response surface methodology. A box-behnken design (BBD) with response surface modeling (RSM) was employed to determine the significance of the various process parameters and their interactions by means of the analysis of variance. After the oxidation process, the removal of polar sulfones from diesel fuel was investigated using chitosan-coated bentonite (CCB). The result showed that 82% removal of sulfur was demonstrated by the system. Thus the outcome of this study clearly demonstrate the effectiveness of utilizing CCB as an adsorbent with high shear oxidative desulfurization in sulfur removal.

# Paper ID-14

## The derivation of dimensionless governing equations for fluidization

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**Abstract:**
In fluidized bed, the fluidization behaviour of particle/powder can vary very drastically with the different velocity, the particles sizes and also the fluid properties such as gases and liquids. Geldart has classified the powders characteristics into 4 groups according to the particles sizes and density. This is generally known as Geldart's powder classification chart. In the classification chart, there are fluidization behaviors that still cannot be clarified yet such as the homogeneous and also bubbling fluidizations. In the bubbling fluidization, bubble behavior is also varies, i.e. fast and slow bubble. A lot of studies about the homogenous and bubbling fluidization have been conducted using the stability analysis. On the other hand, the fast and slow bubbles that appear in a fluidized bed have been studied by Davidson and Harrison using their proposed model and through analysis of the gas flow around a bubble. Numbers of study have been conducted in order to clarify the constitutive mechanism of fluidization behind the differences between the homogeneous and bubbling fluidizations. However, the basic fundamental mechanisms have not been sufficiently clarified yet. In this study, we focused on the nondimensionalization of governing equations. The governing equations for the DEM (Discrete Element Method)-CFD (Computational Fluid Dynamics) coupling model are non-dimensionalized using the method of Hellums and Churchill. The effect obtained with the dimensionless parameters on the fluidization behaviors was also examined. As the results in this study, we have compared the simulation results on dimensionless and dimensional equations. Both have showed the same results and from this we can say that the flow behavior in fluidized bed can be analyzed using the dimensionless expression.

# Paper ID-16

## Effect of microwave heating on casein isolated from tetra pack milk and fresh milk by FTIR

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**Abstract:**
The main objective of present study was to investigate the effect of microwave heating on casein isolated from tetra pack milk and fresh milk by FTIR. Comparative study between two types of heating methods (microwave and conventional) was done between two milk samples (Milk Pak and fresh buffalo milk) both were purchased from local market of Hyderabad, Pakistan. Both the samples were heated at a range of temperature (room temperature, 22oC, 35oC, 42oC, 55oC, 59oC, 70oC, 79oC, 96oC) in microwave oven and by conventional method. All the samples were then analyzed for pH, specific gravity and subjected for isolation of casein. The casein collected from each sample was then analyzed by Fourier Transform Infrared Spectroscopy. We found that pH was remarkably decreased after temperature 22oC and increased after 50oC by both methods. The specific gravity was found to be nearly same at all temperatures. It was explored that peaks 1635 cm-1 and 1615 cm-1 (the diagnostic peaks of amide -1 band) were present in the protein structure. The other temperature intervals gave us different peaks which are as follows: (i)1339 cm-1 is the range of amide (peptide) bond III by the CM at the temperature of 35oC, Amide III is resulting from in-phase combination of C-N stretching and N-H in-plane-bending, with some contribution from C-C stretching and C=O bending vibrations. (ii) 699.71 cm-1 at the temperature of 42oC is the range calcium carbonate, the coagulation of protein is accelerated by calcium carbonate. (iii) When the temperature rise to 55oC in MWM the peak 1096.80cm-1 is found, this corresponds to the stretching vibrations of the phosphate group. In conclusion, the specific gravity and pH are not influenced by microwave heating, only the coil structure of protein is influenced. Casein may undergo a change by which stretching of phosphate bonds occur as indicated by FTIR.

# Paper ID-17

## Enhancement of Biodegradable Polymer Properties by Physical and Chemical Revisited Method

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**Abstract:**
Recently, interested in compound production has moved towards using natural polymers as strengthening due to the environmental advantages. The use of Bio-degradable polymer is worth considering since this will result in fully biodegradable compound. In to evaluate the most appropriate array plastic, one has to know the property of available plastics. Since information tends to be dispersed over several sources and are very rare in comparison to the traditional polymer materials, it is the goal of this article to provide an overview of the most relevant property of the range are biodegradable polymers. A review like the one shown here can provide a helpful guide to establish the best balance between the comparing properties requirements.

# Paper ID-18

## Review of Low-Temperature H2S Sorbents for Desulfurization of Biogas

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**Abstract:**
This review surveys sorbents that remove Hydrogen Sulfide (H2S) from biogas generated at low-temperature ranges from different sources. Biomass feedstocks contain low percentages of protein-derived sulfur that is converted primarily to H2S, as well as small amounts of carbonyl sulfide (COS) and organosulfur compounds during fermentation, gasification, etc. These sulfur species must be removed from the raw biogas before it is used for downstream fuel synthesis or power generation as of their disadvantages such as corrosion, acid rains, and human health problems. Several types of sorbents and ceria have been developed over the last two decades that are capable of removing H2S from biogas at low-temperature ranges. This study has been divided the current sorbents through recent investigations into three main categories; (1) Activated carbons, (2) Metal based materials, and (3) Microporous and mesoporous silica. Further improvement is essential to develop sorbents more suitable for desulfurization of biogas because of their low efficiency, and high price, which present different challenges to eliminate hydrogen sulfide at low-temperature ranges.

# Paper ID-19

## Kenaf As Adsorptive Gas Storage

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**Abstract:**
Kenaf (Hibiscus Cannabinus L.) has been recognised as potential due to its outstanding characteristics, lightweight and porous structure. However, it need a better surface interaction characteristics for gas adsorption and less hydrophilic. The objectives of this study are to modify the surface properties of kenaf and determine the physicochemical properties of the modified kenaf for hydrogen adsorption. Metal hydride has been used to modify kenaf sample in different quantities (10 wt %, 20 wt % and 30 wt %). By modification, the kenaf increased its surface properties and improve the adsorption characteristics. The structural changes of modified kenaf were observed in the field emission scanning electron microscopy (FESEM) analysis. The adsorption capacity results also show the effect of LiBH4 on kenaf sample.

# Paper ID-20

## $CO_2$ removal using mdea/amp in liquid emulsion

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**Abstract:**
The capture of carbon dioxide (CO2) by aqueous alkanolamine is the most cost-effective technology available today. However, some problem such as amine losses, corrosion and low absorption rate arose when using aqueous alkanolamines as an absorbent. To overcome these problems, liquid emulsion was introduced as an alternative for CO2 removal. However, the main concern of using liquid emulsion is the stability. In this study, a formulation containing mixture of blended alkanolamine was used. Methyldiethanolamine (MDEA) and 2-amino-2-methyl-1-propanol (AMP) were used as extractants and were mixed with aqueous sodium hydroxide (NaOH) to form the aqueous phase. Meanwhile, the organic phase consists of kerosene and Span 80 as the surfactants. The emulsion was prepared with a homogenization speed of 10 000 rpm at time interval of eight minutes. The stability and pH of the MDEA-AMP emulsion were determined and the CO2 absorption by the emulsion was measured. Using 4 mL MDEA and 4mL AMP, the stability and pH of the emulsion was 90.15% and 9.56 respectively, and the amount of percentage CO2 removed was 45.58%.

# Paper ID-21

## Development of a rapid, effective method for seeding biofiltration systems using alginate bead- immobilized cells

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**Abstract:**
The antisocial and health problems associated with odours from waste handling sites has led to the design of specialised biofiltration systems which use microorganisms to metabolize malodorous compounds to safer compounds. In order to reduce the pro-longed start-up process of a biofilter, such systems are often seeded with selected microorganisms to facilitate rapid biofilm formation. In order to ease application, these microorganisms can be immobilised by entrapment within three dimensional polymer matrixes such as alginate beads. The bead structure, slow biodegradability and good diffusion properties of beads made with alginate serve as a simple protective layer which limits the exposure of microorganisms to unsuitable conditions. In addition, the beads can also incorporate nutrients which will support the initial cell survival whilst they acclimatise to the new environment. Over time, the biodegradable bead slowly loses its structural stability, thereby releasing entrapped cells to colonise the biofilter media. This research investigates the development of freeze-dried alginate-immobilized cell beads into a commercially viable method to seed biofiltration systems. The process by which alginate immobilized cells progressively colonises, leading to biofilm formation within the structure of the biofilter media will be illustrated by microbiological analyses combined with scanning electron microscopy. The cell immobilisation and freeze drying methodology necessary for increasing the shelf life of the beads, whilst maintaining cell viability, will also be described. Synthesis and modification of palm seed based activated carbon to remove Dibenzothiophene

# Paper ID-22

## Synthesis and modification of palm seed based activated carbon to remove Dibenzothiophene

*Eilham S Moosavi, Ramin Karimzadeh**
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**Abstract:**
This work examines the effects of modification of hydrogen treated activated carbons (ACH) by 65% HNO3 oxidation to two different levels of surface acidity (i.e., oxidation at 25 and 100oC) and copper impregnation on the adsorption of dibenzothiophene(DBT) as refractory sulfur compound in model diesel fuel. For this purpose one mesoporous palm seed based activated carbon was synthesized and then modified. The pore structure and surface properties of the AC samples were characterized by N2 adsorption XRD and Boehm titration methods. The DBT adsorption capacity of the AC samples increases in the order of: oxidized sample at 100oC (ACHO-100)< hydrogen treated sample (ACH) < copper impregnated sample (ACH-Cu+)< oxidized sample at 25oC (ACHO-25). Surface oxidation at 25oC leads to increasing about 30% DBT adsorption capacity. The improved adsorption performance upon the HNO3 oxidation can be attributed mainly to an increase in the acidic oxygen-containing functional groups. At sever oxidation temperature condition (100oC), the adsorption capacity of the activated carbon samples decreases 60% due to pore blocking and porous structure devastating. Cu2O-loaded sample exhibited the high DBT uptake due to more specific interactions, including π-complexation and acid-base interactions between Cu+ species and DBT molecule.

# Paper ID-23

## Development of Reverse Ultrasonic Tomographic Instrumentation System for Monitoring Irregularities on Aboveground Gas Pipeline

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**Abstract:**
This paper presents the development of reverse ultrasonic tomographic instrumentation system to monitor irregularities on gas pipeline surface for aboveground pipe inspection in oil and gas industry. It is very crucial to detect irregularities such as crack or corrosion that may lead to pipeline ruptures which will cause fires and explosion. The developed system is based on the reverse tomographic technique as the object to be imaged is located at the outside layer of pipe, with ultrasonic sensors mounted at specific distance from the object. This research started with the modelling of reverse ultrasonic sensing system that consists of ultrasonic ring design configuration, arrangement of sensors and determination of image area of ultrasonic signal for fabrication purposes. Twenty-eight ultrasonic transceiver sensors are plugged in the ultrasonic ring, where the ultrasonic ring is positioned outside the external pipe surface with a fix distance of 50 mm as modelled. The inspection is based on the detection of ultrasonic signal reflected from the surface or objects to the sensors. Based on the output signal obtained in voltage values, the distance of ultrasonic reflected to the sensor is computed. Several experiments have been carried out to evaluate the capability of the instrumentation system in detecting irregularities on the pipe. There are seven irregularities simulated around the pipe surface. The irregularities are detected based on the output signal and are analysed based on its depth, which is ranging from 0.4 to 3.3 mm. An image of pipe profile with the irregularities existence is then reconstructed. The results indicate that the developed instrumentation system is capable to detect any irregularities at different depth with a minimum of 0.4 mm.

# Paper ID-24

## The Novel Amine – Modified Kenaf as $CO_2$ Adsorbent in Pressure Swing Adsorption (PSA) System

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**Abstract:**
The emission of carbon dioxide (CO2) to the atmosphere is implicated as the predominant cause of global climate change. Currently, adsorption is one of the technologies that able to capture the greenhouse gas. This paper introduced kenaf as a new potential adsorbent for CO2 adsorption. The work involved impregnating the precursor of kenaf with a series of alkanolamines (MEA, DEA and MDEA) to enhance the CO2 adsorption capacity. Initially, 20 wt % of MEA, DEA and MDEA has been impregnated on kenaf via wet impregnation method. CO2 adsorption study is achieved in pressure swing adsorption (PSA) system by passing CO2/N2 mixture in a ratio of 30/70 up to 1.5 bar at ambient temperature. Field emission scanning electron microscope (FESEM) analysis was used to observe the morphological structure of amine – impregnated kenaf and the result indicated that kenaf structure was affected after impregnation of MEA, DEA and MDEA. The presence of these alkanolamines has improved the CO2 adsorption capacity of kenaf as compared to the raw kenaf. The amount of CO2 adsorbed is in the order of MDEA > DEA > MEA. This result could be explained by the pore filling effect due to the difference in molecular size and shape of amines used. Finally, our results exhibited that the amine – impregnated on kenaf could enhance the adsorption capability of kenaf and its capacity in three consecutive adsorption cycles.

# Paper ID-25

## 4,6-Dimethyldibenzothiophene adsorption by activated carbon fiber

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*University of Tehran, Islamic Republic of Iran*
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**Abstract:**
Two hydrogen-treated activated carbon samples (ACFH, ACH) were oxidized with 65% HNO3 at two different levels of surface acidity (i.e., oxidation at 25 and 100 oC). 4,6-dimethyldibenzothiophene (4,6-DMDBT) in single-solute system from n-hexane solution was used as thiophenic compound solution. The surface chemistry and textural properties of all tested adsorbents were characterized by Boehm titration, FTIR and N2 adsorption. Oxidation at 25 oC leads to increasing about 30% thiophenic compounds adsorption capacity. At sever oxidation temperature condition (100 oC), the adsorption capacity of the activated carbon samples decreases 100% due to pore blocking and porous structure devastating. The results indicate that oxygen acidic functional groups of activated carbon are a good candidate with high capacity for removing of the refractory sulfur compounds specially 4,6-DMDBT. Textural properties and surface chemistry significantly influence on the adsorption of three investigated thiophenic compounds. The DBTs molecules with higher aromatic rings and methyl group can be adsorbed on the surface via acid–base and active site interaction mechanism.

# Paper ID-26

## Computational modeling of catalytic systems and adsorbents

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**Abstract:**
The talk includes selected examples of the application of computational chemistry methods to problems, related to catalytic systems and nanoparticles. The calculations were performed with density functional method using different models.

# Paper ID-27

## Synthesis of 3,4-disubstituted coumarin derivatives via ultrasonic conditions

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**Abstract:**
Coumarins are natural compounds with wide application in organic synthesis as acceptors in different organic reactions with nucleophilic reagents and dienophiles in Diels-Alder reactions as well in reactions of [2+2] or [2+3] cycloaddition and as intermediates in the synthesis of products of practical interest. On the other hand, especially important are their antimicrobial, antiviral, anticancer, enzyme inhibition, anti-HIV, and antioxidant activities as well as their influence over central nervous system. A third large area of application of coumarin derivatives are modern technologies They can be applied as excellent luminophores and laser dyes. Coumarin derivatives may be used as ligands for metal complexes and for modification of organic and inorganic supports. The investigations on the chemical behavior of the 3-substituted 2-oxo-2H-1-benzopyranes (coumarins) toward nucleophilic reagents represented them as good acceptor in the 1, 4-addition reactions. Reactions of the 3-substituted coumarins with organomagnesium, and organozinc reagents as well as with Ivanov's reagent were carried out and the corresponding 2-oxochromanes were isolated with good yields. The reactions with their analougs 1,2-benzoxaphosphorine as substrate had the same synthetic progress but in these cases were isolated only two of possible diastereoisomers. The reactions were carried out under ultrasound irradiation and the yields of the target products were higher and the results were accurate and precise. Interestingly nucleophilic addition of halogen subsituted anhydride in the presence of Zn lead to formation of biscoumarins. Condions sugested by us represent a new method for the synthesis of this type of compounds under simple and eco-friendly experimental set up. Acknowledgment: The investigations are financially supported by the Bulgarian Science Fund –Contract № DID 02/23/2009. The authors are grateful to the FP7 Project - Beyond Everest.

# Paper ID-28

## Effect of Feed Loading on Biogas Methane Production in Batch Mesophilic Anaerobic Digesters treating Food Wastes.

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**Abstract:**
Food waste mixture upgraded to carbon to nitrogen ratio 30 was co-digested at different feed loadings of 0.5, 1.5, 3.5 and 5.5gVS/L at batch and mesophilic condition (37oC). Results showed that the biogas methane produced increased with increasing feed loading to the digester. A maximum cumulative biogas methane yield of 0.535L/gVS was attained at feed loading of 3.5gVS/L. Generally it was observed that higher feed loading to digester led to pH reduction and drop in treatment efficiency of digester from 96% to 75%.

# Paper ID-29

## Extraction and Screening of Various Hydrolases from Malaysian Channel Catfish (Ictalurus punctatus) Viscera

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**Abstract:**
Malaysia is a large producer of fish that is estimated to be 1.5million tonnes every year. 35-50% of the fish weight is its viscera, which is usually disposed into the landfills or sea leading to massive environmental problems. However, various hydrolases can be extracted from this highly potential by-product source. In this study, protease, lipase, alpha-amylase and cellulase activities were studied. Protein concentration of the whole viscera of Ictalurus punctatus was 0.798596 mg/mL, protease gives the highest specific activity among the hydrolases (13.57 U/mg), cellulase was (1.43 U/mg), lipase (1.425 U/mg) and the alpha-amylase was (0.689 U/mg).

# Paper ID-30

## Quantifying Uncertainty of Spatial Interpolation of Fine Particulate Matter in Small Regions using Empirical Bayesian Kriging

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**Abstract:**
Since monitoring of fine particulate matter (PM2.5) in the U.S. gained traction in 1999, continuous monitoring has evolved from fixed monitoring to better capture diurnal variations of PM2.5 levels. However, it remains difficult to determine specific PM2.5 levels within small regions (e.g. downtown areas) due to few monitoring stations that provide sparse data that are typically aggregated to cover large areas (e.g. county, state and/or national level) Consequently, several studies have sought to develop deterministic and probabilistic interpolation models that predict PM2.5 levels at various spatial and temporal resolutions. While many studies acknowledge the existence of inherent spatial and temporal uncertainties behind their models, very few go ahead to quantify the resulting spatial implications of said uncertainty especially within a small region. Our study uses a probabilistic model to quantify the uncertainty of diurnal PM2.5 prediction over a small region of approximately 100 square kilometers. Using an empirical dataset of continuous PM2.5 readings collected from a fixed station and hand-held PM2.5 monitoring devices with GPS capability, we conduct interpolation of continuous PM2.5 levels in the downtown area of the town of Keene, New Hampshire. Therein, we employ an interpolation technique known as Empirical Bayesian Kriging (EBK) that uses simulation of various parameters to account for the error resulting from estimating the semivariogram model. Further, we optimize our proposed interpolation model by defining our search neighborhood as the average nearest-neighbor empirical distance of the geo-located sampling points. Consequently, we are able to minimize the standard error of prediction of continuous PM2.5 levels for the small area of Keene and show that not only does the EBK method out-perform other interpolation methods for relatively small datasets, but also the result is a relatively realistic prediction model that includes various uncertainty parameters for subsequent analyses.

# Paper ID-31

## Geopolitical approach to environmental issues in 21 century

*Seyedabas Ahmadi*, Tahmores Heydari Mosello*
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**Abstract:**
From the end of the 20 century on, human environment at the local, national, regional and international level has been endangered more than before. These hazards have appeared in three aspects: decreased and lack of resources, destruction of the resources, and environmental pollution. From a geopolitical perspective, lack of environmental resources or depriving the human beings of living in their favorite place leads to competition and mutual transaction and even in some cases the conflicts between the human groups and political players in different levels. Therefore, considering the power of thinking that human beings have it was expected that human become a power that could improve the valuable environmental criteria, but, on the contrary, it seems that it has increasingly become a powerful force and caused environmental chaos. In this way, today environmental geopolitical issues and problems are no longer considered as a local or even national issue. And considering the interdependence and inseparable relationship between the environment and major humanistic issues including economy, culture, development, politics and its special form, i.e., geopolitics they have become intertwined. And it seems that majority of the environmental issues at any level and even restricted to the local borders of a country are considered as problematic for the whole world and human beings. In this study, we try to consider environmental issues from a geopolitical perspective using library resources and a descriptive-analytical method and explain the threats and challenges in this regard.

# Paper ID-32

## Adsorption of NO and SO2 on the Sn0.5Ti0.5O2 Catalyst Studied by in-situ FTIR Spectroscopy

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**Abstract:**
We have for the first time discovered that using the composite oxides of TiO2-MxOy as catalyst and CO as reductant can effectively realize the simultaneous elimination of NOx and SOx at relatively low temperature and with no need for any pretreatment for activation[1]. Over the composite oxides catalysts, the activity for CO+SO2 reaction is very high and the selectivity of S is 100%. But the activity for CO+NO reaction is low: the conversion of NO is lower than 50%, the selectivity of N2 is nearly 100%. When the catalyst is used for simultaneous reduction of SO2 and NO by CO, the conversions of SO2 and NO are all higher than 90% with 100% selectivities of S and N2. This indicates that in the present of SO2, there is a sepecial active center for CO+NO reaction on the novel catalyst. Over the sepecial active center the reaction follows a novel reaction mechanism. The reaction mechanism of SO2+CO, NO+CO and SO2+NO+CO (simultaneous reduction of SO2 and NO ---- SRSN) reactions on the SnO2-TiO2 catalyst and catalyst active sites were investigated by in situ infrared Fourier transform spectroscopy. The synergism between SnO2---TiO2 and the physicochemical properties of the SnO2-TiO2 solid solution catalyst have also be studied by in-situ FTIR spectroscopy. To resolve these questions is very important for application and theory.

# Paper ID-33

## Production of heterogeneous catalyst for bio-diesel synthesis

*Beenish Shan*, Sarina Sulaiman, Parveen Jamal*
*IIUM Malaysia*
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**Abstract:**
The waste food material namely crab shell, egg shell and fish bone is screened for biodiesel synthesis by tranesterification reaction to determine the source providing the highest biodiesel yield. The solid oxide materials were calcined at 900°C at 2-4hrs to convert CaCO3 to CaO species. Tranesesterification is carried out at 65°C for 4 hrs with varied methanol to oil ratio. It was found that although egg shell, and crab shell gave average biodiesel yields, fish bone provided outstanding results of the three catalysts. This research signifies successful application of waste resources as an emerging prospective for economical preparation of heterogeneous catalyst, developing an unconventional avenue for reusing of this solid waste.

# Paper ID-34

## Optimization of Pineaple Waste Fermentation Process in Continuous Reactor System

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**Abstract:**
The aim of the present study is to investigate the influence of variations in substrate flow rate and supply O2 in fermentation process by utilizing Acetobacter xylinum. The experiments were carried out on a laboratory scale continuous reactor system operated at room temperature , 25OC-27OC, with a pH of 4.5. The parameters analyzed include BOD5, COD, TPC (sel/mL), ash, weight (GSM), fiber length (mm), fines (%) dan cellulose total content. Data analysis showed that those variations influence the nata layer formation. The best result obtained for nata layer is 3 mm with the characteristic of the pulp from nata is cellulose total content values of 62.34%. The values of fiber length and fines are 0.537 mm and 27.25 %, respectively. While the results obtained for removal efficiency of BOD5 is 49.90% and the values of COD is 50%. Treatment variation that gave the best cellulose was at time detention of 12 days with bacteria growth percentage of 80%. The utilization of pineapple waste study as raw material to produce pulp by utilizing Acetobacter xylinum has not yet been established. This preliminary research will contribute to improve the quality of nata de pina layer.

# Paper ID-36

## Surfactant Behaviour in Water; A Monte Carlo Simulation

*Ruzanna Yahya*, Roghayeh Abedi Karjiban, Mahiran Basri, Mohd Basyaruddin Abdul Rahman*
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**Abstract:**
Self-assembly is the spontaneous aggregation of surfactants hold together by hydrophobic interactions in water. An amphiphile consists of both lyophilic and lyophobic moieties with an ability to form aggregated structure or micelles which occurs above the critical micelle concentration (CMC). Molecular dynamics (MD), Monte Carlo (MC), and the hybrid simulation techniques are among the promising theoretical tools to explore the self-assembly and micellization process for several years. Physical properties of the micelles can be predicted by using these tools with a good accuracy from the concentration, the temperature, and the type of surfactant molecules. We used Monte Carlo method to study the behavior of a surfactant model system in aqueous solution. Monte Carlo is a stochastic numerical experiment in which a configuration of the model is chosen randomly. By this, one can physically determine the behaviour of a model system based on sampling technique. Two nonionic surfactants molecules from Brij family of surfactants were selected. These nonionic surfactants are important in nano-emulsions' formulations due to their less toxicity and less irritancy in comparison with other types of surfactants which later on can be used as nano-carriers. Self-aggregation was detected by using a Monte Carlo lattice model. The model was sampled in water at 300K temperature and 1 bar pressure by using different compositions of surfactants based on experimentally determined phase diagram. The total number of Monte Carlo steps was 5 million. The acceptance ratio obtained was ideal for all selected models. The self-aggregation process was examined by using free energy, radial distribution function, and the radius of gyration. Our results confirmed that the shape of the micelles formed could be affected by the composition of surfactants used.

# Paper ID-37

## Development of algorithm for charge compensation of the large nucleoproteins

*Miroslav Rangelov*
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**Abstract:**
One of major problems in molecular dynamics (MD) simulation of large nucleoproteins is uncompensated charge of phosphate groups. We developed heuristic method for ther neutralisation wich is applied on the ribosome. Ribosomes, the universal cellular nano-machines, act as polymerases that translate the genetic code into proteins with high efficiency. It is a complex molecular machine translated the genetic code of its provisional form - information RNA to proteins. The key role of the bacterial ribosome makes it an important target for antibacterial agents. Due to limitations of X-ray methodology all available ribosome structures contain a lot of missing monomers and are unsuitable for molecular dynamics. For this reason a new whole ribosome structure (E.Coli) was constructed. Starting from most completed available PDB structures we constructed our initial Ribosome model. To obtain a full ribosome structure a new heuristic algorithm is developed. According to this algorithm if there is even a low intensity X-ray map available for the missing monomers it has been used for its placement and positioning. If there is no X-ray map with good enough quality the KEM map is used. When KEM and X-ray maps are of insufficient resolution for positioning of the monomers they are placed by hand and are optimized by Coot FF according to Ramachandran plot minima. After the process of addition of missing monomers the ribosome structure were relaxed by MD. The resulting full ribosome structure is still unsuitable for all atoms MD because of the many charged groups it contains. This is because the ribosome is mainly composed of RNA chains leading to a huge amount of negatively charged phosphate groups in the PDB X-Ray Structures. In nature they are neutralized by Na+, Mg2+ ions and a limited amount of positively charged amino acid residues incorporated in the polypeptide chains. For neutralization of these groups a heuristic algorithm for adding counter ions in big nucleoproteins as the ribosome unit has been developed and the charged groups in the ribosome structure were effectively neutralized using mono and divalent ions according to their environment. The neutralized structure equilibrates with all atom MD within several ns. Due to necessary expertise from different research fields the method was developed in cooperation between several groups within the frame of the National Center of Supercomputer Applications, Sofia, Bulgaria: M. Rangelov and S. Markov from Bulgarian Academy of Sciences, and P. Petkov, P. Petkov, L. Litov and G. Vayssilov from University of Sofia, Bulgaria. The work on these topics was supported by Bulgarian Science Fund and computer time is provided by Bulgarian Supercomputer Center.

## Paper ID-38

# Surfactant Behaviour in Water; A Monte Carlo Simulation

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**Abstract:**
Self-assembly is the spontaneous aggregation of surfactants hold together by hydrophobic interactions in water. An amphiphile consists of both lyophilic and lyophobic moieties with an ability to form aggregated structure or micelles which occurs above the critical micelle concentration (CMC). Molecular dynamics (MD), Monte Carlo (MC), and the hybrid simulation techniques are among the promising theoretical tools to explore the self-assembly and micellization process for several years. Physical properties of the micelles can be predicted by using these tools with a good accuracy from the concentration, the temperature, and the type of surfactant molecules. We used Monte Carlo method to study the behavior of a surfactant model system in aqueous solution. Monte Carlo is a stochastic numerical experiment in which a configuration of the model is chosen randomly. By this, one can physically determine the behaviour of a model system based on sampling technique. Two nonionic surfactants molecules from Brij family of surfactants were selected. These nonionic surfactants are important in nano-emulsions' formulations due to their less toxicity and less irritancy in comparison with other types of surfactants which later on can be used as nano-carriers. Self-aggregation was detected by using a Monte Carlo lattice model. The model was sampled in water at 300K temperature and 1 bar pressure by using different compositions of surfactants based on experimentally determined phase diagram. The total number of Monte Carlo steps was 5 million. The acceptance ratio obtained was ideal for all selected models. The self-aggregation process was examined by using free energy, radial distribution function, and the radius of gyration. Our results confirmed that the shape of the micelles formed could be affected by the composition of surfactants used.

# Paper ID-39

## Characterization of Air Pollution Episodes by PTR-MS Triggered Sampling Coupled with GC/MS Analysis

*Jia-Lin Wang*, Chung-Kung Lai, Hwa-Kwang Yak*
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**Abstract:**
Toxic or foul air pollutants have aroused major public concerns in Taiwan, especially for residential areas peripheral to industrial parks, as manifested by the increasing number of complaints filed to local governments. Therefore, the ability to instantaneously detect relevant compounds from a large pool of volatile organic compounds (VOCs) at a given industrial park is pivotal to emission source investigation. Due to the illusive nature of pollution episodes, in-situ monitoring in or near industrial parks with rapid response to key compounds appears to be a logical solution. Until now, although gas chromatography-mass sepctrometry (GC-MS) has been the preferred choice for VOC analysis due to its strength in compound identification and quantification, it requires long analysis time,rendering it unsuitable to capture and characterize illusive pollution events. On the other hand, proton transfer reaction – quadruple mass spectrometry (PTR-QMS) is a powerful tool for real-time monitoring of ambient VOCs with extremely high sensitivity (1 ppb) and speed (~1 sec). However, the major drawbackof PTR-QMS lies in its unit mass resolution which limits its ability to identify complex gas mixtures. Hence, combining the strengths of both PTR-QMS and GC/MS for their sensitivity, speed and compound identification capabilities would be an ideal way to characterize illusive episodes. To complement the two instruments, the PTR-QMS was not only as a measurement instrument, but also served as a triggeringdevice to active sampling flasks to collect episodic air samples. Target ions specific to a selected industrial park were chosen by PTR-QMS for detecting pollution episodes and,at the same time, to trigger flask sampling when target ion signals surpass prescribedalarm levels. Subsequently, the in-lab GC/MS analysis was used for detailed analysis of more than 100 compounds in the flasks, which together with the instantaneous data of PTR-QMS, were used to characterize the composition of episodic plumes.

# Paper ID-40

## Abatement of Fluorine inside Small Particle Fluidized Bed using Aspen Plus Simulation

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*National Institute of Technology, Rourkela India*
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**Abstract:**
Simulation of a Fluidized Bed Reactor is carried out using Aspen Plus in order to find out the minimum conditions necessary for the abatement of Fluorine from a gaseous mixture obtained mainly from fertilizer, semi-conductor and petroleum industries containing Fluorine, Nitrogen and other gases when it is reacted with some particulates of small sized iron particles inside the Fluidized Bed Reactor. The formation of products will be in solid form as FeF2 and FeF3 with minor amount of Fe thereby indicating the abatement of F2. The bed hydrodynamics and the reactions are studied and is then applied to the Aspen Plus user interface assuming chemical equilibrium where the total Gibbs energy of the system had its minimum value. The modeled data are compared with the literature data where the feeds are 99% pure. The simulated results are found to be in fair agreement with those reported in the literature.

# Paper ID-41

## Phase Behavior of Ionic Liquid with Thiophene based Binary system Predicted using COSMO-RS model.

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**Abstract:**
In this work the COSMO-RS model algorithm was derived from the modified rachford rice method. It could be more helpful to investigate the phase behavior of binary systems with the help of Ab initio method calculation at 6-31G* basis set. For benchmarking a total of 30 systems out of which 4,7,8, and the 10 system belonged to type I,II,III,and IV LLE diagrams respectively. The average value of the root mean square deviation for the type IV systems which is encountered in IL's systems was found to be 4.89% by our developed COSMO-RS model. After successfully bench marking, COSMO-RS was used to predict solubility of binary system involving Non-IL's and IL's systems are: Benzyl ethylamine + Glycerol system (Type-I),Nitro methane + Cyclohexane system (Type-II), Dipropylamine + Water system (Type-III),1,2-ethanediol + Thiophene system (Type-IV), 1,2-ethanediol + Thiophene system (Type-IV),[1,2-DMIM][Salicylate] + Thiophene (Type-IV),and [EMIM][NO3] + Thiophene (Type-IV).A total of 15 cations, which including imidazolium, pyridinium,pyrrolinium,quinonium,and azolium along with 27 anions were used for generating 405 binary LLE systems involving thiophene. However, our predicted COSMO-RS values of 1-Ethyl-3 methylimidazolium thiocyanate ([EMIM][SCN]) ,1-Butyl-3 methylimidazoliumthiocyanate ([BMIM][SCN]) and 1-Hexyl-3 methylimidazolium thiocyanate ([HMIM][SCN]) were seems to be similar with reported experimental values by Domanska et al.[16].Further the immiscibility gap at 298.15K was determined and compared for various IL's.It was found that 1-Butylpyrrolidinium, 1-Octylquinolinium, 1-Octylpyridinium and 1-Octyl-3-methylimidazolium based cations most suitable for thiophene extraction from any liquid mixture.