## 1671<sup>st</sup> Conference INDUSTRIAL CHEMISTRY 2018



 $17^{\mbox{\tiny th}}$  International Conference on

**Industrial Chemistry and Water Treatment** 

May 21-22, 2018 | New York, USA

# Poster Presentations

 $\mathsf{Prove 53}$ 

# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## D-TiO<sub>2</sub>/ZnO-degradation of contaminants present in residual water using TiO<sub>2</sub>/ZnO catalysts

Berenice Angel Hernandez Benemerita Autonomous University of Puebla, Mexico

Degradation of contaminants present in residual water using  $TiO_2/ZnO$  catalysts (D- $TiO_2/ZnO$ ): It is an experimental work which aims to degrade the contaminants present in the water from a municipal wastewater treatment plant. This objective is achieved through the use of UV radiation and  $TiO_2/ZnO$  catalysts. The catalysts used were synthesized using the sol-gel method. The sol-gel method was chosen for the synthesis because this method achieves a high homogeneity and purity of the materials besides presenting a great thermal stability. Once the catalysts were obtained their characterization was carried out by the methods of X-ray diffraction, scanning electron microscopy and energy dispersive spectroscopy. Degradation tests are carried out on the wastewater with the catalysts and an 850mL batch photoreactor composed of a medium pressure mercury vapor lamp which emits ultraviolet radiation with a region between 200-400nm. To follow up the photodegradation, samples were taken and analyzed in a UV spectrophotometer. Physico-chemical, microbiological and genotoxicity analyzes are carried out before and after photodegradation to compare the results and verify that the degradation has been successful. The results of the tests showed an evident decrease in the color, turbidity, solids, heavy metals, chemical oxygen demand and biological demand of oxygen present in the residual water sample.

#### Biography

Berenice Angel Hernandez is currently pursuing her Master's degree in Benemerita Autonomous University of Puebla, Mexico. She has published one paper and realized a stay of investigation in the PSA, Spain.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

### Application of Chlorella vulgaris to wastewater for reuse

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The accelerated growth of the population worldwide has led localities to a greater consumption of natural resources. Overpopulation also requires quality improvement. Industrialization, urbanization and daily consumption have limited the availability of water in many parts of the world, so in some populations, it is necessary to reuse wastewater that is subject to one or two phases of a treatment process, resulting in water poor quality that generates problems on human health. In addition to the above, the present work studies the capacity of metabolism and absorption of phosphorus, nitrogen and heavy metals present in the waste water of the treatment plant of the state of Puebla using *Chlorella vulgaris* algae. This was carried out by bioassays at different concentrations of residual water (Witness, 25%, 50%, 75% and 100%). The test that showed the best characteristics was 100%, this sample was centrifuged to separate the organic matter and later the water was placed in a photoreactor, it was made to react with UV light, hydrogen peroxide and ozone. The content of heavy metals present in the bioassay was determined by atomic absorption. To know the quality of the water treated with this type of technology, the acute toxicity was analyzed by *Daphnia magna* and the anomalies were determined in the cellular mitosis in *Allium sativum*. It should be mentioned that the general water parameters were measured at the beginning and end of each representative stage for a complete analysis.

#### **Biography**

Celeste Solis Martinez has completed her studies in Food Engineering from the Benemerita Autonomous University of Puebla, Mexico. Currently, she is pursuing her Master's in Environmental Sciences.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Identification of genotoxicity in bioindicators produced by wastewater used for agricultural irrigation

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**P**opulation growth, industrial development, intensified agricultural production and the number of contaminants incorporated into the environment have deteriorated the water compartments, it is necessary to develop strategies to reduce and prevent their contamination. In some types of wastewater, products resulting from the biological treatment process (non-biodegradable) may have significant toxicity and high genotoxicity. Genotoxicological effects may manifest at different levels, from subcellular structures or enzyme systems, to whole organisms. The unicellular electrophoresis/Comet assay (EC) and micronucleus are sensitive methodologies, available, cheap and applicable to any cell type to measure DNA strand breaks in individual cells considered as assays indicative of premutagenic lesions. The evaluation of abnormal cells was performed in producers using treated wastewater for agricultural irrigation. The presence of nuclear and micronuclei abnormalities in the identified cells was classified in relation to their nuclear form by observing degenerative nuclear changes related to cellular toxicity. Among the nuclear abnormalities detected in the producers prevail the condensed and binucleated cell nuclei, without observation of more than six micronuclei per thousand cells counted; however, tests on bioindicators (*Allium sativum* and *Vicia faba*) will be carried out to confirm genotoxicity levels generated by the compounds present in the wastewater.

#### **Biography**

Perez-Nava Jessica has completed her MSc from Benémerita Universidad Autónoma de Puebla. Currently, she is pursuing her Doctoral program in the same university. Her research areas include: photochemical treatment of wastewater, genotoxicity and microbiological tests. She has published two scientific papers and has made academics mobilities in Mexico and abroad.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Catalytic wet air oxidation for water purification

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The generation of hazardous waste waters from a variety of industrial processes poses a serious environmental threat. Catalytic wet air oxidation (CWAO) is a growing economical and environmentally friendly process for the removal of toxic organic compounds found in such wastewater streams. Using a continuous 3-phase trickle bed reactor, this project focuses on the complete oxidation of phenol as model organic pollutant. Of the catalysts screened, platinum/silicon carbide proved the most successful, in terms of activity. An explanation is proposed for the increased reaction rates seen when using hydrophobic catalyst supports such as SiC; the presence of a 'surface gas envelope' on hydrophobic supports allows for a secondary mass transfer route of oxygen from the gas phase to the catalyst surface, prohibited by more common hydrophilic catalysts. Investigations were carried out to further optimize the silicon carbide catalysts, and improve mass transfer limitations, with the overall aim of reducing the high energy requirements associated with CWAO, and thus the overall cost and environmental impact.

#### **Biography**

Korrin Saunders has completed her Master's in Chemistry at Cardiff University, and is currently involved with the Centre for Doctoral Training (CDT) program in Catalysis at Cardiff University, University of Bristol and the University of Bath. As part of the CDT, she has obtained a Master's in Research and is currently in her final year of her PhD. Her PhD works are within the Cardiff Catalysis Institute and the School of Chemical Engineering at the University of Bath.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Gold nanoparticles assembled on multilayer graphene sheets for surface enhanced Raman spectroscopy of glucose and related organic pollutants

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The small normal Raman cross-section of glucose is considered a major issue for their detection by surface enhanced Raman spectroscopy (SERS) for medical applications, such as blood glucose level monitoring of diabetic patients and evaluation of patients with other medical conditions since glucose is a marker for many human diseases. Similarly, organic contaminants such as toluene suspended in drinking water require detection and removal. In this work, we report the use of commercial multilayer graphene sheets as substrates on which gold nanoparticles are chemically assembled by citrate reduction. The results show that these substrates are capable of providing SERS enhancement factors up to 1010 with a detection limit to 10-8 M in aqueous solutions of glucose. The SERS performance on graphene substrates are many orders of magnitude higher compared with results on gold coated chemically etched Klarite\* silicon substrates. The glucose spectra over a wide range of concentrations in the 400-1500cm-1 fingerprint region were recorded with a Thermo Scientific DXR Raman microspectrometer using 785nm laser wavelength, 10mW laser power and a 50x microscope objective. The intensity of the 1340cm-1 line of glucose in particular varied linearly with glucose concentration and can be used as a calibration for samples of unknown concentrations. Chemometric methods were used to provide improved spectra at very low concentrations. The role of fractional charge transfer effects from the graphene substrate to glucose that could provide secondary enhancement of the spectra will also be evaluated. Similar preliminary results on toluene suspended in water related to water contamination will also be presented.

#### **Biography**

Laila Al-garni has received her Master's degree in Chemistry from Saudi Arabia at King Abdul Aziz University in 2009. She has started her job in 2008 as Teaching Assistant, then promoted as Lecturer in 2009. She is pursuing her PhD in Physical Chemistry from New Jersey Institute of Technology under the direction of Prof. Zafar Iqbal, where she used Raman spectroscopy for detection of glucose at very low concentration (pharmaceutical and biofuel sensing application).

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## 17<sup>th</sup> International Conference on Industrial Chemistry and Water Treatment

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## Control fouling in membrane distillation

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Membrane distillation (MD) is a technology that designed to remove the salt particles, minerals and other contaminants from sea, brackish or wastewater to produce pure water. The process exhibits higher than 99% salt rejection from the brine water. However, like other membrane processes, membrane fouling is one of the major concerns in MD that reduces the performances of the process significantly. The primary aim of this study was to reduce the fouling by using different antiscalants materials. These active antiscalants interact with the fouling materials and helps to prevent and remove the deposition of the salt clusters from the membrane surfaces to maintain a consistent performance. The use of antiscalant materials was observed to be beneficial in maximizing the overall yield and reducing the time of operation.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## A long-term aerosol prediction model based on a bi-directional long-short term memory neural network

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Which increasing of interests in aerosol for national environmental crisis, prevention of aerosol becomes a major issue for human-being health. As the ecosystem vulnerability becomes clear, the need for long-term aerosol prediction has been attracted. Since it is known that the amount of aerosol is highly related to pollutants such as CO, SO<sub>2</sub>, NO, and so on, the accuracy of long-term aerosol prediction can be increased by exploiting the relation between pollutants and aerosol levels. Therefore, this paper proposes a long-term aerosol prediction model based on a bi-directional long-short term memory (B-LSTM) network, which is a well-known deep neural network technique applied to time-series data. The proposed model is composed of two layers of the B-LSTM network. The lower layer is designed to predict a pollutant rate for up to 3-hour by using the correlation between pollutants and aerosol. The upper layer of the B-LSTM network is for predicting a PM10 rate up to 24-hours by using the lower layer outputs. Here, the B-LSTM network is trained using actual pollutant data collected on an hourly basis for 30 years (from 1987 to 2016) of 15 different industrial locations of South Korea. The prediction accuracy of the lower layer of the B-LSTM network achieved 77.4% for 3-hour prediction of pollutants such as CO, SO<sub>2</sub> and NO. In addition, the prediction accuracy of PM10 from the upper layer of the B-LSTM was evaluated by measuring the root-mean-squared error (RMSE) between actual and predicted. As a result, the RMSE averaged over 15 locations was measured as about 13.77% for 24-hour PM10 prediction.

#### **Biography**

Inyoung Park is currently pursuing her PhD in the School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology, South Korea. She has received her BS degree in Computer Application from the Bangalore University in 2015. Her current research focuses on speech signal processing and climate change modeling based on deep neural networks.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

#### Bacterial isolation capacity to metabolize organic waste from residual water

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W ater pollution is an environmental problem; the waters are accompanied by organic matter, nutrients and trace amounts of metals. The physicochemical treatments allow partial removal of the organic load; however, the costs are high, therefore it is advisable the use of other processes as the biologic. Contaminated rivers represent an interesting source of microorganisms capable of degrading different substrates, considering candidates for isolation and purification processes used in contaminated water. The strategy of bioremediation technologies is the use of different metabolic pathways and increased degradation of native processes to eliminate or reduced the contaminating substances. The isolates were monitored in medium with different substrates (carbohydrates, proteins and glycerol). Nineteen bacterial isolates from the three monitored water bodies were obtained, the percentage of capacity to assimilate strains with different carbohydrates varied depending on the compound, 100% of the strains degraded dextrose and sucrose, degraded 86% starch, 66% casein and none of the isolates showed hydrolysis of gelatin and lipase production. Results are in close relation to the place where these bacteria were isolated; as different levels of contamination may influence the bacteria present characteristics to adapt to the use of a wide range of carbohydrates. Although the degradation of pollutants in nature is often the result of the activity of a microbial consortium rather than a single organism, the potential degrader consortium depends on the potential that microorganisms present individually in their interaction with specific pollutants, for this reason have isolated autochthonous capacity to remove organic matter is a pathway for future use.

#### **Biography**

Rivera-Tapia A has completed his undergraduate and graduate studies at the Benemérita Autonomous University of Puebla, Mexico obtaining his Doctorate in Environmental Sciences in 2009, he began working at the same university from 1997 to date. He currently directs Master's and Doctoral theses in the areas of Environmental Science and Technology. His research areas focus on environmental problems and microbiological tests. He has published more than 10 articles related to the topic of wastewater characterization within the city of Puebla; and participated in more than 15 national and international congresses on topics focused on the area of Environmental Sciences.

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## 1671<sup>st</sup> Conference INDUSTRIAL CHEMISTRY 2018



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Accepted Abstracts

# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Synthesis of water treatment chemicals adaptable to rural clean and drinking water technology

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Statement of the Problem: A cross section of rural communities in Africa are plagued by diseases many of which are water borne or attributable to the quality of drinking water accessible to such communities. Access to clean freshwater is very necessary to human life and for industries like steel, copper, food, paper, petroleum, chemical or mineral processing industry (Willey et al., 2008). Due to its good solvent property, water tends to dissolve a broad spectrum of substances from the environment. These include toxins and toxicants emanating from various forms of domestic, agricultural, industrial and other anthropocentric activities including hazardous substances from natural phenomena like earthquakes and volcanic eruptions. Contaminated waters are highly undesirable as they constitute a significant source of disease and worldwide death (Willey et al., 2008). Polluted water usually contains organic matter such as hydrocarbons and their derivatives, inorganic matter such as clay, sand, acids and bases, heavy metals such Pb<sup>2+</sup>, Cu<sup>2+</sup>, Ni<sup>2+</sup>, Al<sup>3+</sup> and pathogenic microbes like Vibro cholerae, Entamoeba histolytica and Salmonella typhi which are causative agents for water-borne diseases like cholera, dysentery and typhoid (Willey et al., 2008). Most rural communities in Africa including Cameroon cannot afford sophisticated water treatment systems and require cheap and simple operable techniques to treat water for domestic purposes and related uses. The goal of all water treatment technologies is to remove turbidity as well as chemical and pathogenic contaminants from water sources in the most affordable and expedient manner possible (Ray & Jain, 2011). The purpose of this study was to synthesize water treatment chemicals which can easily be adapted to domestic water treatment in rural community water systems in order curb rampant spread of water borne diseases typical of rural communities in Africa. The water treatment chemical is environmentally friendly due to its propensity to biodegradation (Tripathy & Singh 2001).

**Materials & Methods:** This bonafide water treatment chemical was produced from Gum arabic and polyacrylamide through graft copolymerization using ceric ammonium nitrate as a catalyst for the reaction. Gum arabic was purchased in powdered form which is the organic component of the product that confers biodegradable properties and acts as the back born for graft copolymerization. The graft copolymer was blended with *Moringa oleifera* seed extract which has antimicrobial activity (Lar et al., 2011, Orhevba et al., 2013).

**Results:** The results obtained showed that the percentage yield of the graft copolymer is a function of both the initiator and monomer concentrations. The grafted copolymer was characterized by IR spectroscopy. The IR spectral data for pure Gum arabic and that of Gum arabic–grafted polyacrylamide indicate that grafting actually occurred. The flocculation properties of the product were good, figure 1.

**Conclusion & Significance:** The successful grafting of polyacrylamide onto Gum Arabic will enhance the search for materials transformation through chemical derivatization with attendant expansion of their spectra of application.

**Recommendations:** More research should be done into the use of simple potent water treatment chemicals which will help to alleviate the plight of the rural populace with attendant amelioration of public health and economic advancement.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## An exact analytical solution for thermal response in biological tissues under therapeutic treatments incorporating an actual initial condition

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The genesis of the present research paper is to develop a revised exact analytical solution of thermal profile of 1-D Pennes' bioheat equation (PBHE) for living tissues influenced in thermal therapeutic treatments. In order to illustrate the temperature distribution in living tissue both Fourier and non-Fourier model of 1-D PBHE has been solved by 'Separation of variables' technique. Till date, most of the research works have been carried out with the constant initial steady temperature of tissue which is not at all relevant for the biological body due to its living cells. There should be a temperature variation in the body before the therapeutic treatment. Therefore, a coupled heat transfer in skin surface before therapeutic heating must be taken account for establishment of exact temperature propagation. This approach has not yet been considered in any research work. In this work, an initial condition for solving governing differential equation of heat conduction in biological tissues has been represented as a function of spatial coordinate. In a few research work, initial temperature distribution with PBHE has been coupled in such a way that it eliminates metabolic heat generation. The study has been devoted to establish the comparison of thermal profile between present approach and published theoretical approach for particular initial and boundary conditions inflicted in this investigation. It has been studied that maximum temperature difference of existing approach for Fourier temperature distribution is 19.6% while in case of non-Fourier, it is 52.8%. We have validated our present analysis with experimental results and it has been observed that the temperature response based on the spatial dependent variable initial condition matches more accurately than other approaches.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Determination of personal care products and pharmaceuticals in river sediments, KwaZulu-Natal, South Africa

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A quantitative method is described for ultrasonic-assisted solid-phase extraction (SPE) followed by GC-MS after derivatization for the simultaneous analysis of personal care products and pharmaceuticals (PCPPs); propyl paraben, triclosan, caffeine, carbamazepine and chloramphenicol. Ultrasonic combined with centrifuge were used to extracts sediments samples collected from Mgeni and Msunduzi River. An SPE procedure was used for clean-up and to concentrate selected compounds from diluted aqueous extracts. Final extracts were derivatized with BSTFA and analyzed with GC-MS in selected ion monitoring (SIM) mode. The recoveries of the analytes ranged from 66% to 108%. The method detection limits were 0.08–1.82ngg-1 and quantification limits 0.42–5.51ngg-1. The proposed method was applied in the evaluation of two rivers over three month period in KwaZulu-Natal, South Africa. All targeted compounds were present in the environment at concentration level between not detected to 174ngg-1. To our knowledge, this is a first report on the simultaneous determination these PCPPs by GC-MS in Africa.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Statistical approach to the optimization of biodiesel production from Jatropha curcas oil

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*Jatropha curcas* oil (JCO) is a plant-based non-edible feed stock that can be modified in order to enhance its use as biodiesel. In this work, optimization of biodiesel production from Jatropha curcas oil was investigated. Biodiesel was produced via a bath catalyzed transesterification reaction of the oil with methanol. This process was optimized by the application of two-level-four factor ( $2^4$ ) Factorial design and response surface methodology (RSM) requiring 16 experiments. A linear model of the form y=84.86+4.98x1 - 3.50x2 - 2.50x3+3.10x4+5.13x1x2 - 0.71x1x4+3.02x2x3+0.13x2x4 - 2.31x1x2x4 was obtained to predict the yield of biodiesel (y) as a function of reaction time (x1), Natt catalyst concentration (x2), methanol to oil ratio (x3) and temperature (x4). A modified statistical model comprising of all significant factors obtained by multiple regression predicted that the highest yield of the JCO based biodiesel was 94.03% at the following optimization rules x1=2.50 hrs, x2=1.1; x3=3.1 and x4=70°C. Also, there was significant interaction between x1x2, x2x3 and x2x4. Gas chromatographic analysis of the JCO biodiesel identified myristate and palmitoleate as the major fatty and ethyl esters. The model has been found to describe the experimental range studied adequately.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Passive biosorption of heavy metal ions to plant-derived materials: Investigations of responsible chemical interactions

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Waste water remediation using biosorption of toxic heavy metal ions by plant materials provides many desirable characteristics. Selective removal of heavy metal ion pollutants in the presence of benign metal ions offers significant advantage for biogenic sorbents relative to commercially synthesized materials. Unfortunately, implementation of these materials for waste water treatment has been limited by their inherent chemical complexity. Gain an understanding of the responsible fundamental chemical interactions has been the focus of our research for several years. We initially selected for these studies, materials derived from the plant Datura innoxia. Because of the chemical complexity of this material, the application of multiple, orthogonal probes were required to study metal ion biosorption to these materials. We have utilized an arsenal of techniques involving luminescence spectroscopy with extraction of thermodynamic parameters governing these interactions. Carboxylate moieties were initially identified as primarily responsible for metal ions sorption. These chemical interactions involved both formation of surface complexes and the involvement of electrostatic attraction to the negatively charge biomaterial. In later work, these studies were expanded to include variations in tissue types from both the same and different plant species. The impact of these findings on the potential of biosorbents for contaminated water treatment will be discussed.

# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Effect of different types of washes on the fabric strength of denim

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E xperimental design (DOE) economically maximizes information; we deliberately change one or more process variables (looms) in order to observe the effect, the changes have on one or more response fabric properties. In DOE, obtained data can be analyzed to yield valid and objective conclusions. An experimental design is lying out of a detailed experimental plan in advance and maximizes the amount of information that can be obtained for a given amount of experimental. Fabric of 36 inches having following weaves was used. 3/1 twill, warp cotton (10.5 den), weft Lycra (16 spandex \* 70 den) Ends per inch 86, picks per inch 52 and washes process includes stone wash, rinse wash, bleaching and enzyme wash. Once the samples were ready, they were subjected to tensile and tear strength tests, for these two kinds of samples were considered. One washed fabric samples of warp direction type and other type of the samples was weft direction. Then five samples from each were considered for tensile and teat strength tests and enzyme wash. Maximum breaking load of the enzyme washed fabric sample was 42 kg.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Ozone initiated inactivation of *Escherichia coli* and *Staphylococcus aureus* in water: Influence of selected organic solvents prevalent in wastewaters

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zone absorption, stability, and reactivity in water are critical distinguishing factors for efficiency in either micropollutants abatement or microbial inactivation. These are also largely, a function of the nature of the dissolved organic matter in the water matrix. In the present study, the influence of four water-soluble organic solvents commonly discharged from industrial lines into wastewater systems viz; ethanol, methanol, ethyl acetate and dimethyl sulfoxide (DMSO) on the ozone facilitated inactivation of Escherichia coli (ATCC 25218) and Staphylococcus aureus (29213) in water was explored. An ozone bubblingtime dependent absorption (up to 12min) and decomposition rate monitored spectrophotometrically in the presence of 2.5% and 5% concentrations of each organic solvent with their consequent effect on bacteria inactivation were determined. The inactivation kinetics were described by the Efficiency Factor Home model. Relatively, higher residual concentrations of absorbed ozone per unit bubbling time were obtained for the solutions of ethyl acetate and DMSO in comparison to methanol and ethanol. Ozone stability was significantly enhanced in solutions containing DMSO or ethyl acetate which was characterized by a lower pseudo- first order decomposition rate constant in DMSO ( $k_a$ =3.381x10<sup>-2</sup>M<sup>-1</sup>s<sup>-1</sup>) and ethyl acetate ( $k_a$ =4.45 x10<sup>-2</sup>M<sup>-1</sup>  $^{1}s^{-1}$ ) solutions and in contrast with methanol (k<sub>1</sub>=1.13 x10<sup>-1</sup>M<sup>-1</sup>s<sup>-1</sup>), where the rate of decomposition was rather accelerated. The faster absorption and stability of ozone in ethyl acetate and DMSO corresponded with an observed increase in the log inactivation of E. coli and S. aureus by approximately 2-folds in relation to methanol at comparable conditions. These findings are significant to the determination or prediction of the lifetime of ozone for efficient disinfection or pollutants oxidation in industrial wastewater treatment systems.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

### Adsorption and decomposition of methanol on Ru-Pt/boron-doped graphene surface: A DFT study

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The decomposition reaction of methanol is currently attracting research attention due to the potential widespread applications of its end products. In this work, a periodic density functional theory (DFT) calculations have been performed to investigate the adsorption and decomposition of methanol on Ru–Pt/boron doped graphene surface. It was found that methanol (CH<sub>3</sub>OH) decomposition through O-H bond breaking to form methoxide (CH<sub>3</sub>O) as the initial step, followed by further dehydrogenation steps which generate, formaldehyde (CH<sub>2</sub>O), formyl (CHO), and carbon monoxide (CO), is found to be the most favorable reaction pathway. The results showed that CH<sub>3</sub>OH and CO groups prefer to adsorb at the Ru-top sites, while CH<sub>2</sub>OH, CH<sub>3</sub>O, CH<sub>2</sub>O, CHO, and H<sub>2</sub> groups favor the Ru-Pt bridge sites, showing the preference of Ru atom to adsorb the active intermediates or species having lone-pair electrons. Based on the results, it was found that the energy barrier for CH<sub>3</sub>OH decomposition through the initial O-H bond breaking is less than its desorption energy of 0.95eV, showing that CH<sub>3</sub>OH prefers to undergo decomposition to CH<sub>3</sub>O rather than direct desorption. The study provides in-depth theoretical insights into the potentially enhanced catalytic activity of Ru–Pt/boron doped graphene surface for methanol decomposition reactions, thereby contributing to the understanding and designing of efficient catalyst at optimum condition.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Green synthesis of silver nanoparticles using *Moringa oleifera* fruit extract and its application to the photocatalytic degradation of methylene blue

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Green synthesis of stabilized silver nanoparticles (AgNPs) using aqueous extract of *Moringa oleifera* fruit is presented in this study. The reduction of Ag+ to Ag0 was confirmed by the formation of reddish-brown solution and the appearance of surface plasmon resonance band at around 400nm. The optimum conditions of the synthesized AgNPs were at 30% extract concentration, pH10 and contact time of 7 days. Further, the stable AgNPs were characterized using UV-Vis spectroscopy, Fourier-Transform Infra-Red (FTIR) spectroscopy and Transmission Electron microscopy (TEM) analysis. TEM images revealed that the average diameter of the synthesized AgNPs was 31.3±13.7nm. Photocatalytic degradation of methylene blue was measured spectrophotometrically by using silver as nanocatalyst under visible light, UV light and solar irradiation. Results showed that the biosynthesized AgNPs were found to be notable in degrading methylene blue under solar irradiation of nearly 40% decolorization at 6 hour of exposure time.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Kinetics and mechanism of periodate oxidation of two ternary nitrilotriacetate chromium (III) complexes involving histidine and aspartate co-ligands

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The oxidation of  $[Cr^{III}(HNTA)(Hist) (H_2O)]$ - and  $[Cr^{III}(HNTA)(Asp)(H_2O)]$ - (NTA=nitrilotriacetate, Hist=L-histidine and Asp=DL-aspartate) by periodate in aqueous medium has been studied spectrophotometrically between 15.0 and 35.0°C under pseudo-first-order conditions,  $[IO_4]$ - [complex]. The rate increases over the pH range 3.40-4.45 in both cases, but the two complexes give different rate laws, in aqueous solutions,  $[Cr^{III}(HNTA)(Hist)(H_2O)]$ - is oxidized by  $IO_4$ - according to the following rate law:  $d[CrV^I]/dt = (k_1K_2 + k_2K3K_1/[H+1))[IO_4-][Cr^{III}]T/{1+ (K_1/[H+1)) + (K_2 + K_1K3/[H+1))[IO_4-]}$ . The other case is  $[Cr^{III}(HNTA)(Asp)(H_2O)]$ - the derived rate law is given by equation: Rate= $k_1K_2[Cr^{III}]T/{1+ ([H+1]/K_1) + K_2[I^{VII}]T}$ . Electron transfer, outer-sphere and inner-sphere mechanisms have been discussed. The nature, properties, chemical behavior and different species in aqueous solutions of periodate have been reported. A literature survey on the oxidation of organic and inorganic compound in aqueous solutions and in aqueous organic solvent was reported. The nature of  $\alpha$ -amino acids and their metal complexes have been briefly discussed, it is clear that  $[Cr^{III}(NTA)(Asp)(OH)]_2$ - may be the reactive species, an inner-sphere process may be still accommodating through replacement of coordinated  $H_2O$  in two species by IO4-. The rate of reaction increases with the increasing of complex concentration and ionic strength. The thermodynamic activation parameters were calculated, and we propose that electron transfer proceeds through an inner-sphere mechanism, via coordination of IO4-to chromium (III). A common mechanism for the oxidation of some to chromium(III) complexes by periodate is proposed by an excellent isokinetic relationship between and values for these reactions.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Physic chemical properties of water samples collected from urban and rural areas of district Peshawar

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The purpose of this study was to investigate different water samples from rural and urban areas and to find either the quality L of water lies within the allowed range or not. Drinking water of different areas like urban, rural, industrial areas and home drinking water of Warsak road are analyzed through different techniques. We checked different parameters in drinking water such as pH, conductance, temperature and hardness of water, chlorides, silica concentration and heavy metals. The average pH of water of urban area is 8.2, water of rural area has average pH of 8.01, for water of industrial area is 9.3 and that for drinking water of Warsak homes is 9.2. The pH is analyzed through pH meter of Model No. PH 2602. The average conductance of urban water is -061 my, for rural area is -083 my, for industrial area is -066 my and that for drinking water of Warsak road is -060mv. The other parameter is hardness of water which is analyzed through simple titration. The average value of hardness of urban water is 0.59 mg of CaCO3/5 ml, for rural sample is 0.65 mg of CaCO3/5 ml, for industrial sample is 0.77 mg of CaCO3/5 ml and that of drinking water of Warsak road is 0.39 mg of CaCO3/5 ml. The concentration of chlorides in most of the urban drinking water is 29.99 mg/l, and of rural samples have average value of 49.99 mg/l. The industrial sample possess the concentration of chloride 14.39 mg/l and of drinking water of Warsak road is 20.98 mg/l. Silica are found in trace quantity in which urban water sample have average value of 1.7\*10-18 ppm. The average mean for rural sample is 2.4\*10-18 ppm. Effluent sample of industrial area have the average mean of 1.6\*10-18 ppm. We have checked two heavy metals (e.g. Nickel and Lead) in drinking water of different areas. Nickel concentration in urban sample like Su2 and Su42 has values of 0.01 and 0.004 mg/L. Industrial and drinking water of Warsak road have absence of Nickel concentration. The lead concentration is found in four samples namely Es4, Sr41, Sr61 and Sr2 which have the values of 0.03 mg/L for Es4, 0.02 mg/L for Sr41, 0.02 mg/L for Sr61 and 0.04 mg/L for Sr2. These heavy metals are detected through Atomic Absorption Technique.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Adsorption of iron, lead, cadmium and zinc ions as a function of soil particle size

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The adsorption level of lead, iron, cadimium and zinc were examined as a function of soil particle size. The clay soil sample used for the experiment was collected from a defunct brick industry located at Ire-Ekiti in Ekiti State. The experiment result present the concentration of adsorbed metal ions using 40ppm solution on each of the soil particle size (150pm, 300 $\mu$ m, 400 $\mu$ m and 1180 $\mu$ m) at a pH of 10 and time of 36 hours. In conclusion, the research work has shown that adsorption of iron, lead, cadmium and zinc would occur significantly mostly when soil of small particle size is used.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## An efficient and straight forward synthesis of 1, 4-dihydropyridines under solvent free conditions

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Now a day's researcher is focused on finding out alternative source of energy that works on green chemistry principles. Chemical reactions under solvent free conditions offers enhanced selectivity, efficiency, easy to manipulation and often avoid toxic, harmful and volatile solvents. Solvents-free approaches involve grinding, ultrasonic irradiations, microwave irradiations or catalysis by inexpensive and recyclable catalysts. Further heterocycles containing nitrogen have significance and most of them carry out some physiological functions in living cells as well as used in industrial and pharmaceutical fields. Among the various heterocycles, 1,4-dihydropyridines belong to a class of nitrogen containing heterocycles having a six-membered ring. Synthesis of these compounds is a keen area for researchers and attracts attention due to their noteworthy medicinal and biological activities. They are used in pharmaceutical (as antimalarial, vasodilator, anesthetic and anticonvulsant) dye and photo industries. They are also used for treatment of cardiovascular disorders and chemosensitizer as well as antitubercular agents. Observing the biological and medicinal properties of these 1,4-dihydropyridine derivatives, an efficient, simple, straightforward reaction involving ethyl acetoacetate, arylaldehyde and ammonium acetate in specific ratio in the presence of ammonium sulfate as catalyst has been described. The catalyst is easily available and recyclable. The method is advantageous in terms of excellent yields and short reaction times.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Bioinspired synthesis of biomolecule-derived fluorescent nanodots from natural amino acids with enhanced photo-stability, biocompatibility and cellular uptake

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Natural amino acids possess different side chain R groups which make them excellent precursors for programmable synthesis of biomolecule-derived fluorescent nanodots (bio-dots) with desired properties. In order to establish the material design rules, 20 amino acids-derived bio-dots were synthesized via hydrothermal treatment and comprehensively characterized. We discovered that the properties of the bio-dots are determined by their unique side chain functional groups. Amino acids such as Arg, His, Asp, Asn, Ser and Thr with reactive side chains including amine, hydroxyl and carboxyl functional groups give rise to bright bio-dots with quantum yield >15%. The length of the side chains is also critical in determining the final morphology (e.g., nanodot, nanowire or nanomesh) and consequently the photoluminescent properties of the bio-dots. It is worthy to note that hydroxyl-containing amino acids (i.e., Ser and Thr) form highly photostable bio-dots with negligible intensity reduction upon UV exposure. Selective mixing of specific amino acid precursors (such as Ser with Arg) leads to the formation of hybrid bio-dots which exhibit enhanced photostability photo-stability with significant red-shift in their emission wavelength. Furthermore, cell studies demonstrate that the bio-dots displayed outstanding biocompatibility and excellent intracellular uptake, which are highly desirable for fluorescence imaging applications. As such, bioinspired synthesis of bio-dots provides a versatile route for customizable development of nanoscale biomaterials by design.

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# **Industrial Chemistry and Water Treatment**

May 21-22, 2018 | New York, USA

## Characterization and treatment of alcoholic effluent wastewater using chemical methods

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The molasses-based distilleries are one of the most polluting industries and pose a serious environmental and health concerns with a deep dark brown colored wastewater/spent wash. Physicochemical characterization of the effluent was investigated before and after the spent wash was entering to waste treatment plant unit. The treatment was done by chemical methods using activated carbon and ferric chloride. At optimum parameters, COD, TDS and TSS of the effluent samples were reduced by 52, 38.6 and 36%, respectively by adsorption process using activated carbon. By coagulation process; the COD, TDS and TSS of the effluent samples were reduced by 40.8, 29 and 37%, respectively using ferric chloride as a coagulant. From the result, it was concluded that treatment of distillery spent wash using chemical methods was not sufficient to treat the distillery waste to the required level and it might be better to integrate biological and chemical methods of treatments.

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