PAKISTAN INSTITUTE OF CHEMICAL ENGINEERS

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Abstract Book

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ii. Publishes literature, research journal, newsletter etc., to educate and update its members and society with the current activities of the Institute.
iii. Work for the uplift of the Chemical Engineering profession.

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Catalysis and Chemical Reaction Engineering / Heat Transfer

Furfural synthesis over zeolite-based catalysts

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Abstract: Lignocelluloses and hemicellulose present in the biowaste/biomass is valuable and cheap feedstock for the production of various green chemicals and energy fuels. It can not only help to reduce environmental impacts of waste but also can contribute to the future energy demand. Development of stable and recyclable solid acid catalysts in the efficient valorisation of hemicellulose to produce furfural and derivatives. The concept boosts the utilization of bio-waste into value added chemicals. Rice is one of the important kharif crops of Pakistan. Additionally, it is one of the important export articles of the country, contributing 2.40% in gross domestic product (GDP) in the national economy (approximately, In Pakistan, rice is produced on 2.883 million hectors area and yearly cultivation of rice is 7.213 million tonnes). Rice husk which is usually burnt in the rice mills in Pakistan as fuel can be utilized to generate revenue by converting into furfural and derivatives over acid catalysts.

In the present work, three zeolite based catalysts are evaluated for conversion of rice husk to biomass at atmospheric pressure. The activity of in house synthesized/modified catalysts is studied by varying reaction conditions such as time, temperature, and feed/acid ratio. The catalysts were characterized using XRD, SEM, and N2-adsorption techniques to find out its pore size, surface area and morphology. Purity and yield of furfural was obtained by GC-FID analysis. Zeolite beta with post aluminium impregnation gave highest yield of bio-oil (60.3 %) with 92% selectivity towards furfural which is comparable with literature reported values. Stability of catalyst was also studied by evaluating activity of the regenerated catalyst. The decrease in activity was less than 5% for five runs of experiments.

Investigating the effects of Inherent Alkali and Alkaline Earth Metal Catalysis on Biochar Gasification

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Abstract: Gasification is an important route for the clean utilization of low-rank fuels e.g. peat, lignite, or biomass etc. The synthesis gas produced during the process has a high calorific value and can be used for electricity generation in reciprocating engines or turbines, for domestic cooking as well as heating. Low-rank fuels have alkali and alkaline earth metallic species (AAEM) dispersed even at the atomic scale. The biochar-O_2 reaction and biochar-H_2O reaction are considered fundamental reactions in the gasification process. The char-O_2 reaction oxidises carbon in an exothermic reaction and supplies energy to drive the endothermic char-H_2O reaction, which produce valuable synthesis gas. Understanding the mechanisms and the role of AAEM species during these reactions is critical to the development of advanced biomass gasification technologies. The present study aims to gain insights into the mechanisms and kinetics of the biochar-H_2O and biochar-O_2 reactions using raw-wood and treated wood in order to understand the role of AAEM species. For this purpose, the raw wood samples were acid-washed to remove AAEM species present in the raw wood samples. Both type of samples were gasified in H_2O and O_2 atmospheres in a fluidised-bed reactor to produce synthesis gas. The components of the synthesis gas were monitored with a quadrupole mass spectrometer. The kinetcis of the biochar gasification was developed using raw-wood and acid-washed wood samples. This paper shows that the nature of the active sites during gasification of raw-wood is different comapred with those in the gasification of acid-washed wood. This paper will discuss the changes in active sites during the char conversion in O_2 and H_2O atmospheres for both raw-wood and acid-washed wood samples.

Photocatalytic degradation of cancerous pollutant (Bisphenol A) from aqueous waste using Bismuth based nanomaterial

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Abstract: Nanotechnology is becoming ubiquitous in everyday life due to the characteristic properties of nanomaterials and their extended applications in numerous fields. The growing interest in wastewater treatment using nanomaterials makes it an emerging technique in this area. Bisphenol A, an identified Endocrine Disruptor Compound, known for its adverse effect on human health is used as a starting material in the production of epoxy resins and polycarbonate plastics. Increased consumption of plastic goods, prompting the BPA usage as well as discharge in the environment. Different studies on BPA removal include adsorption, coagulation, ozonation, biodegradation, etc. In this work, visible-light-driven photocatalytic degradation of BPA is carried out in the presence of pristine Bismuth oxide (BC0) and Cu_2O deposited Bismuth oxide (BCx, x=0.5, 1, 1.5, and 2) synthesis followed by hydrothermal and ultrasonication methods. The BC0 and BC1 were characterized by XRD, DRS, FTIR, SEM, and EDX. The distinctive peaks by XRD confirm the formation of bismuth oxide. The light absorption of samples in the visible region was depicted by DRS. SEM results reported the sheet-like morphology for bismuth oxide with tiny particles of Cu_2O attached to its surface. Decomposition of BPA under visible radiation is tested for all the composites as well as pristine bismuth oxide with the optimum degradation results achieved for BC1, i.e., up to 96%. Finally, the findings of this work are providing a new sight for the photocatalytic treatment of organic-contaminated wastewater by bismuth-based nanocomposites in the presence of visible light radiations with high performance.

Keywords: Nanomaterials, Photocatalysis, Bismuth oxide, hydrothermal, visible-light radiation.

Synthesis and Catalytic property of Chiral Pd@Cu nanomaterials with of Purine Nucleotides

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Abstract: As key components of DNA, nucleobases, nucleosides, and nucleotides have emerged as a viable building block for the creation of functional nanomaterials. The use of biomolecules as templates in the synthesis of nanomaterials provides a good technique for controlling and regulating their morphologies and other properties. In this study, we demonstrate the formation of different chiral morphologies of Pd@Cu nanoparticles by employing purine nucleotide as a Chirality and morphological inducer. Furthermore, we study the effect of purine nucleotides on the preparation of chiral Pd@Cu, nanoparticles with spherical, platelets and hexagonal morphologies. In the presence of Purine nucleotides (ATP, GTP), Pd@Cu nanoparticles were successfully constructed. Transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and chiral dichroism (CD) spectra were used to characterize the produced chiral metallic nanoparticles. The Pd@Cu chiral nanoparticles were used for a variety of applications due to their controlled size and shape. The research provides a potential approach for production of nano materials with controllable morphologies and various applications in Catalysis, optoelectronic devices, sensing or imaging, chemosensory, energy materials and bio-probes.

Synthesis of 1-Tetradecene via Thermal Decomposition of Castor Oil

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Abstract: 1-tetradecene is a primary ingredient for the paint industry. 1-tetradecene is linear alpha olefins (LAO) or normal alpha olefins (NAO) are olefins or alkenes. Due to by linearity of the hydrocarbon chain and the double bond position, these are distinguished by the other mono-olefins. 1-Tetradecene is used in the production of mercaptans, oxo-alcohols, amines and amine oxides, alkylated aromatics, alpha olefins sulfonates, synthetic lubricants, epoxides, tanning oils, and as drying oil. Currently, 1-tetradecene is produced synthetically by Oligomers which is formed by using a modified Ziegler ethylene chain growth technology. However, this process is carried out at high pressures i.e., 13.8 – 27.6 MPa. The thermal cracking of castor oil is another way to produce 1-tetradecene (obtained from the seeds of Ricinus Communis) which are acetylated by acetic anhydride in the presence of p-toluenesulphonic acid. In the present study, a detailed comparison is carried out to produce 1-tetradecene by the above mentioned two processes including ethylene oligomerization and thermal cracking of castor oil. For this purpose, the simulation models of both processes were developed using a process simulator i.e., Aspen Plus. The base cases of these simulation models were also validated by the date from the literature. The simulation results show that the castor oil process is more efficient and economical as its yield consist of 99% of pure 1-tetradecene while the yield of the ethylene oligomerization process is found to be 95%. Further, thermal cracking of castor oil can be carried out at lower pressures i.e., 105 – 195 kPa. In addition to this, the catalyst (Ni-Sn) required for thermal cracking of castor oil is less expensive than the catalyst (Triethylaluminium) required for the ethylene oligomerization process. In this study, a detailed comparison will be presented highlighting the effects of various operating conditions on the production of 1-tetradecene and optimum conditions will be suggested.

A Rapid Method of analysis of insulating Oil through non-destructive Spectroscopic techniques

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Abstract: Material testing is very important to track the progress of any material. The testing techniques should be rapid, easy to analyze, non-destructive. While testing the material the sample should not get impurities and not be damaged or destroyed. One of the vital materials that need to be analyzed is insulating oil. As transformers are the most important component of the power system. Failure in the transformer can cause a big financial loss so a timely inspection of the transformer is necessary. The service life of a transformer can be determined by the condition of the insulating oil. In this research, we have studied the insulating oil through a rapid non-destructive technique, i.e. Fourier Transform Infrared spectroscopy (FTIR) and ultraviolet and visible (UV-Vis) spectroscopy. For this purpose, the oil was aged in the presence of insulating paper in an oven at 130˚C for different periods, and the oil was checked through FTIR and UV-Vis after every 48 hours. From the change in intensity of the peaks of FTIR between 1700 cm-1 to 1600 cm-1, Carbonyl and aromaticity indices have been calculated from the area under the curves at a specific wavenumber which reflects the deterioration of insulating oil. Further, the UV-Vis spectrum intensity between 200nm-400nm will help to analyze qualitatively the quality of insulating oil. These non-destructive techniques are rapid, inexpensive, and also carry a lot of information as compared to the traditional method, through which we can decide about the state of the oil.

Keywords: Insulating oil; Non-destructive techniques; FTIR; UV-Vis; Carbonyl index; Aromaticity index.

Computing, Control, and Process Systems

Simulation and optimization study for CO2 and H2S removal from natural gas using MDEA and Sulfinol-M with Piperazine as activator

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Abstract: The presence of both H_2S and CO_2 in natural gas lower its quality which leads to the development of reliable and novel techniques required to capture both H_2S and CO_2 from sour natural gas. In the present work, process simulator Aspen Hysys V12 is used to simulate and optimize the gas sweetening process in steady state. The simulation study was conducted to evaluate the utilization of Sulfinol-M with piperazine solvent to replace the aqueous amine solvent (MDEA) currently used in the sour gas treatment plants. The simulation of the Sulfinol-M with piperazine process demonstrates less energy consumption, and lower the losses of solvent versus in comparison to MDEA solvent, and thus can be considered as alternative solvent due to its higher efficiency for removal of sour gases from natural gas.

Development and Simulation of a Methanol Production Plant from CO_2 Hydrogenation using Captured CO_2 considering Cost Effectiveness

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Abstract: The reutilization of CO_2 to produce value-added chemicals and fuels can help to solve the environmental problems associated with CO_2 emissions generated by burning fossil fuels. One of the most important products that can be produced from CO_2 is methanol, the process is a part of the so-called "Methanol Economy". Methanol is not only a quality liquid fuel that can be used in motor vehicles, but it is also a precursor of many industrially important chemicals. The CO_2 is captured by chemical absorption from the flue gases of a thermal power plant. The Hydrogen is produced by water electrolysis using carbon-free electricity through Polymer Electrolysis Membrane fuel cell method. The Methanol plant provides 30-36% of the thermal energy required for CO_2 capture, reducing considerably the costs of the capture. As the methanol synthesis is an exothermic process, the research is about the Design, Modeling, and Simulation of the reactor to efficiently manage the reaction heat as planned; keeping cost effectiveness in consideration.

Keywords: CO_2 reutilization, global warming, methanol synthesis, hydrogenation, cost.

Sorption enhanced gasification of biomass in a circulating fluidized bed to produce H_2 rich syngas - An Investigative Study on Aspen Plus

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Abstract: Biomass offers a promising future in the production of synthetic fuels and reducing greenhouse gas emissions. Gasification of biomass is a thermochemical and 'carbon neutral' process whereby solid biomass is converted into synthesis gas. Synthesis gas can be used for power generation as well as for chemical synthesis like methanol, dimethyl ether, gasoline, etc. A prime factor in gasification, which is not fully considered, is the cost associated with Air Separation Unit (ASU). Without ASU, conventional processes result in the dilution of syngas with N_2, resulting in a decrease in calorific value as well as larger-sized downstream equipments. Dual circulating fluidized bed gasification ensures elimination of ASU without affecting syngas composition. This coupled with sorption enhancement through CaO produces H_2 rich syngas, which is best suited for chemical synthesis. For this purpose, the simulation model of the dual circulating fluidized bed gasification process was developed using a process simulator i.e., Aspen Plus. The base case was also validated by the data taken from the literature. We have found the use of CaO raised the H_2 composition to as high as 70%. Further, the high pressure favored CH_4 yield while also raising the gasification temperature. Steam ratio not only affected H_2 yield but also CO_2 production. This study will investigate the effects of the equivalence ratio, sorbent requirements, operating parameters, and their mutual dependence on the gasification process and the optimum conditions will be suggested.

Natural gas condensate stabilization with CO_2 removal through steady state optimization processes

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Abstract: Objective of this research work is to model the efficient stabilization unit in term of available energy and on-spec stabilized condensate product. Natural gas condensate liquids (NGL) need to be stabilized by removing lighter hydrocarbon gases and impurities such as CO_2 before sending to storage and transportation to refinery. Stabilized NGL have vapor pressure determined as Reid Vapor pressure, nearly 7 psia which shows light components do not evolve as a separate gas phase. Stabilization along with CO_2 removal process has been performed through fractionation method by heating and pressure reduction using steady state and dynamic Hysys software. Fractionation has been proven to be an efficient method among different available techniques. Different process configurations around exchanger, column and reboiler such as, straight through and split flow for feed/bottom heat exchanger towards the column, Nitrogen stripping in the column and heat recovery around reboiler has been studied based on utilities available for stabilization and CO_2 removal process. Parametric studies such as, impact of increase in CO_2 concentration and temperature at inlet of stabilizer inlet flash separator, ramp up/ ramp down study and dynamic simulation for PID controller has been performed to analyze process performance parameters such as, RVP and CO_2 at rundown air cooler, and heat duties for exchangers and initial startup/shutdown condensate stabilization unit behavior. Actual plant data results are used to validate the Hysys simulation values for the accuracy of condensate stabilization unit model. The process has good performance in respect of reducing the RVP, facilitating energy conservation, operating safety, and increasing economic benefit.

Design and Modeling of a Novel Reactor-Heat Exchanger System for the Dehydrogenation of Methylcyclohexane

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Abstract: The methylcyclohexane-toluene-hydrogen (MTH) system is considered as one of the potential solutions for the successful conception of a hydrogen-based economy. The success of the MTH system is principally dependent on the dehydrogenation reaction of methylcyclohexane which is highly endothermic and occurs at rather high temperatures. To accommodate the highly endothermic nature of the dehydrogenation reaction of the MTH system, a suitable configuration of the reactor and heat exchanger system with a suitable catalyst of known kinetics is required to design and optimize for commercial applications of the MTH system. Since a large sum of heat energy is required to carry out this reaction and considerable temperature drops occurs in the radial direction of a conventional fixed bed reactor, lower rates of conversion are achieved, and the performance of the reactor is deeply affected. A highly efficient reactor design is therefore required that is capable of providing the heat energy at a sufficiently fast rate. In the present study, an intensified reactor-heat exchanger design is proposed and simulated using the reaction kinetics (for 1.0wt%Pt/Al_2O_3 catalyst) developed previously in our group. Mathematical modeling of the reactor system is carried out and the corresponding partial differential equations are solved following the explicit finite difference method. Parametric study of the reactor system is undertaken to observe its response to the various operating conditions. The optimum conditions for the operation are then worked out.

Simulation of Chemical Vapor Deposition Reactor

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Abstract: Chemical vapor deposition (CVD) is one of the most effective methods of producing carbon nanotubes. Multiwalled carbon nanotubes (MWCNTs) developed through chemical vapor deposition (CVD) has a relatively low production rate compared to the many of the other methods employed for its synthesis. The final yield is determined by the reaction conditions of CVD reactor. The process parameters need to be optimized for realizing a high yield. The deposition rate of multiwalled carbon nanotubes depends mainly on various parameters such as temperature, pressure, hydrocarbon concentration, catalyst purity, xylene/ferrocene feed rate and inlet velocity of carrier gas. One of these parameters i.e., inlet concentration of hydrocarbon feed is studied previously. Recent studies show that parameters like reaction temperature, xylene/ferrocene feed rate and inlet velocity of carrier gas can also contribute to increasing the overall deposition rate of CNTs effectively just like inlet concentration of hydrocarbon. The major problem is to develop a model of such system and to simulate that model against different reaction temperatures and inlet velocity of hydrocarbon/carrier gas. The developed computational fluid dynamics model of chemical vapor deposition reactor is simulated against real reaction conditions to determine the most suitable operating conditions for getting increased production rate of multiwalled carbon nanotubes. In our model, two gas-phase reactions and four surface reactions are considered. The rate constants of the surface reactions are determined using the inverse technique based on the measured tail gas concentrations. The predicted production rate agreed well with the experimental data, validating our model.

Thermal Modelling of a High-power Lithium-ion Cell using Equivalent Circuit Modelling Approach

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Abstract: Electric vehicles (EVs) and hybrid electric vehicles (HEVs) help minimizing environmental deterioration and reducing burden on fuel market. EVs are expected to supplant internal combustion engine (ICE) vehicles in near future. Majority of the EVs and HEVs use lithium-ion batteries as a power source due to higher voltage and longer cycle life. A major drawback associated with lithium-ion batteries is their temperature sensitivity. Higher temperatures degrade battery performance and reduce cycle life. Moreover, elevated temperature could cause fire or explosion. Managing temperature within an optimum operating range is essential for EV power modules. Modelling and simulation is a convenient and effective tool for thermal characterization of lithium-ion batteries. Physics based lithium-ion battery models are too expensive computationally and hence cannot be used on a system level. Equivalent circuit models on the other hand are robust and suitable for onboard application. In present work a three-dimensional equivalent circuit model is developed to predict thermal response of a commercially favoured high-power lithium-ion cell under different operating conditions. ANSYS FLUENT® is used to solve the model equations. Simulations are carried out at low to moderate current loads (1C, 2C, and 3C). Simulation results obtained under constant current (CC) discharge demonstrate excellent accord with the experimental data at 1C and 2C discharge rate. Although at 3C discharge rate the model shows a slight divergence but still it gives a reasonable approximation of the cell response.

Keywords: Electric Vehicle; Hybrid Electric Vehicle; Equivalent Circuit model; Lithium-ion battery.

Simulation of lithium-Ion battery half cell using pore network modelling approach

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Abstract: Lithium-ion batteries (LIB) are the prominent source of energy in electric vehicle industry and consumer electronics such as cell phones and laptops. Enhancing the performance of these batteries using experimental and modelling techniques will not only assist reducing conventional fuel resources but also reduce environmental pollution. In modelling domain, pore scale modelling is usually performed using direct numerical simulation (DNS) to study structural performance relationship of porous components in LIB's. Due to high demand of computational resources used in DNS it becomes infeasible to mesh a big porous domain using computational resources available to average user. On the other hand, pore network modelling is a computational efficient approach that can simulate big porous domains without losing structural heterogeneities of porous structures. This approach allows investigating localized effects on pore to pore or particle to particle basis to help remove structural bottlenecks in porous components. Present work focuses on developing a pore network modelling framework to study galvanostatic discharge behavior of lithium-ion battery half cell. Three-phase pore networks were extracted from 3D tomograms of $Li(Ni_{0.5}Mn_{0.3}Co_{0.2})O_2$ (NMC-532) cathodes having different thickness. To analyze structural-performance relationship various structural properties were extracted using PNM approach. Developed PNM framework was used to simulate discharge curves at different C-rates and gave a good agreement with published results. The structural heterogeneities of porous phase revealed important insights about structural bottlenecks in porous cathodes. Lastly, computational performance of the developed pore network modelling framework was studied at different C-rates and a significant gain in simulation time was observed. The developed framework opens a new avenue to study structural effects on porous electrodes on the overall performance of cell at very less computational cost and allows removing bottlenecks of transport and kinetics resistances faced during fast charging/discharging of lithium-ion batteries.

Khan, Z. A., Agnaou, M., Sadeghi, M. A., Elkamel, A. and Gostick, J. T. Pore Network Modelling of Galvanostatic Discharge Behaviour of Lithium-ion Battery Cathodes. *J. Electrochem. Soc.* **168**, 070534 (2021).

Modeling and simulation of a coupled reactor for hydrogen production in an integrated fuel cell power system

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Abstract: Pakistan is amongst the top countries facing severe energy shortfall causing the economy to drain at an alarming rate. Sustainable energy is essential to cope with this crisis and curtail greenhouse gas (GHG) emissions. Industrial and transportation sectors heavily dependent on fossil-based fuels. Unstable fuel market and GHG induced global warming combined with climate change drive the world to explore alternative sources of energy that are abundant as well as clean. Hydrogen is designated as a fuel of future, thanks to its higher heating value and zero direct emissions. Fuel cells directly convert hydrogen into electrical energy. Fuel cell power modules require hydrogen that conventionally was shipped and stored on the site. Due to its very low density and explosive nature, transportation and handling of hydrogen is a challenge. Modern fuel cell power modules have integrated reformer along with a combustor referred to as coupled reactor. SOFC operates at very high temperature so exhaust gases contain a significant amount of thermal energy which can be utilized within the integrated reforming process. In addition, anode off-gas (AOG) from SOFC contains unreacted hydrogen which can be utilized as fuel in an integrated combustor thereby increasing combustor efficiency. In the present work, a 3D model of an integrated coupled reactor is developed and implemented into the computational fluid dynamics (CFD) simulation package ANSYS FLUENT®. Main objective of this work is to prove the concept of enhancement in combustor performance by utilizing AOG from SOFC as a supplementary fuel in the combustor. With the use of AOG, simulation results reveal a considerable increase in combustor temperature and heat dissipated to the reformer side. This work also includes model parameterization study as well as identification of appropriate kinetic models for combustion and reforming reactions taking place in the coupled reactor. Detailed simulations are carried out to optimize performance of the coupled reactor in an integrated combustion-reforming-power-generation (CRP) setup.

Keywords: Coupled reactor, Hydrogen, Solid Oxide Fuel Cell, Computational Fluid Dynamics, Reforming.

CFD modeling and parameter optimization of anode-supported solid oxide fuel cell (SOFC)

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Abstract: In contemporary world, industries rely mostly on fossil-based fuels, which have limited supply and serious consequences for the environment. This prompted researchers to explore other environment friendly energy sources like fuel cells (FC). FCs are electrochemical devices that convert chemical energy of fuels directly to electrical energy. Solid oxide fuel cells (SOFCs) are inexpensive with high temperature performance capabilities. SOFCs utilize transition metals at both the cathode and anode. Wide range of fuels can be handled like biogas and syngas, which are very productive, and seems to have no effect on the environment. SOFC technology has not been fully commercialized. But extensive research is underway to optimize design and operation parameters of SOFC. Computational fluid dynamics (CFD) is an inexpensive and efficient tool to investigate SOFC performance. In present work, a 3D model is developed and implemented into a commercial CFD package ANSYS Fluent® Fuel Cell addon module. A single channel geometry is developed using ANSYS Design Modeler®. Geometry domain is discretized using high quality Finite Volume (FV) structured mesh. Kinetic and thermodynamic parameters are optimized using experimental data. Kinetic parameter includes reference exchange current density while thermodynamic parameter includes entropy and reaction enthalpy. Different exchange current densities from literature are applied at anode and cathode catalyst layer or triple phase boundary (TPB) while ignoring thermodynamic energy loss. Once the reference exchange current density is optimized, effect of entropy change is investigated. User defined functions (UDFs) written in C-based codes are used to apply heat source terms. Once the parameters are optimized, power characterization of the cell is done using detailed simulations. Hence present model shows promise in performance optimization studies and can further be used for design and optimization of SOFC stacks and modules.

Keywords: SOFC, anode-supported, renewable energy, energy conversion.

Computational fluid dynamics simulation of indoor air flow

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Abstract: The present research demonstrates the comparison of the numerical simulation results of two Computational Fluid Dynamics (CFD) programs ANSYS CFX and ANSYS FLUENT for a 2D base case model of indoor air flow under turbulent flow conditions. The purpose is to develop a better basic physical understanding and to select the suitable CFD program for the development of the 3D transient multicomponent simulation model to simulate the emissions propagation. The specifications of the indoor air flow model under turbulent flow condition were taken from the literature. The geometry was created using ANSYS Design Modeler and the mesh generation was carried out in ANSYS Meshing. The comparison of the velocity contours from the two programs shows that the velocities predicted by these programs are almost the same. All the simulation results are consistent with the results reported in the literature.

Conventional and Non-conventional Energies

Evaluation of energy potential and methane generation from Municipal Solid Waste (MSW) of Gujranwala city (Pakistan)

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Abstract: Waste landfill sites are the source of methane generation which is biggest contributor to global warming. The main purpose of this study is to determine the concentration of methane gas from Municipal Solid Waste (MSW) at the site of Bakhrewali in the Rahwali Cantonment area, Gujranwala city, Pakistan and to estimate the amount of energy that could be recovered from the MSW site. The waste samples were collected to analyze the composition, energy content, and concentration of methane. The results from the characterization of MSW showed that the main component of Bahrewali site, Gujranwala MSW is organic waste, that is made up of 65 % by wt. of the waste. Methane concentration from sites 1, 2 and 3 were recorded to be 118.45, 35.32, 48.26ppm methane/g waste. The calorific value of the waste samples was measured to be 13.45, 12.24, and 11.01MJ/kg. These findings affirm that the formation of methane gas at the waste sites could be used for energy recovery. Also, the calorific value of the waste samples suggests that these samples can be combusted and be utilized as feedstock for electricity generation.

Keywords: Gujranwala city, Rahwali Cantt, Municipal solid waste, Methane gas, Calorific value.

Thickness Optimization of Non-Toxic Germanium Based Perovskite Solar Cell Using SCAPS-1D

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Abstract: Perovskite solar cells being efficient and cost-effective are grabbing the photovoltaic industry with their great electronic and optical properties. In the present study, the performance of lead-free and non-toxic cesium germanium tri-iodide (CsGeI3) based perovskite solar cells with C60 as Electron Transport Layer (ETL) and CuI as Hole Transport Layer (HTL) is simulated using SCAPS-1D software. The thickness of absorber layer, ETL and HTL are optimized to get the maximum power conversion efficiency (PCE). Interface layers are also added in-between the layers to obtain more realistic results. The maximum Power Conversion Efficiency (PCE) of 15.02%, Fill Factor (FF) of 85.88%, a short circuit current density (Jsc) of 19.799 mA/Cm2 and open-circuit voltage (Voc) of 0.8831V were obtained.

Keywords: Perovskite; Solar cells; SCAPS; Germanium; Non-toxic.

Investigation of synergistic/inhibitive effects during Biochar Gasification in the mixture of CO_2 and H_2O

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Abstract: Energy from biomass is renewable, sustainable, and reliable. Gasification is a thermochemical process for the efficient conversion of low-rank fuels (e.g., biomass) into syngas, which can serve as a basic building block for the synthesis of many other organic chemicals. The biochar-H_2O reaction is an important reaction to produce syngas during gasification. CO_2 is a greenhouse gas and there are growing concerns for the utilization of CO_2 due to its adverse environmental impacts. The gasification process can serve a particular advantage when CO_2 is utilized as a gasifying agent to produce CO-enrich syngas during the process. Therefore, it is important to investigate the kinetic behavior of biochar gasification in the mixture of CO_2 and steam to understand the effects of the presence of CO_2 during steam gasification. The present study has focused on the gasification of mallee wood in carbon dioxide and the mixture of steam and CO_2. A fluidized bed reactor was used for gasification and the product gases were analysed using a quadrupole mass spectrophotometer. The apparent activation energy and the apparent pre-exponential factors were calculated at various char conversion levels. We found that the apparent activation energy and the apparent pre-exponential factor values were different during gasification in CO_2 compared with those values in the mixture of CO_2 and steam. We also observed the kinetic compensation phenomena in both gasification atmospheres with the inhibitive effect of CO_2 gas on char reactivity during H_2O gasification. This implies that CO_2 and H_2O compete for the same active sites on the biochar surface during gasification in the mixture of CO_2 and H_2O. This paper will discuss the changes in the kinetic behavior as well as changes in the kinetic compensation effects to gain mechanistic insights into biochar gasification in the presence of steam as well as CO_2.

Biotechnology, Bioeconomy, and Bioengineering

Production of fuel graded Ethanol by Fermentation starting from Molasses

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Abstract: From by product (Molasses) of sugar industry to produce Biofuel (Ethanol) through fermentation. Anhydrous ethanol (ethanol with less than 1% water) can be mixed with gasoline in shifting amounts up to immaculate ethanol, and most modern-day gasoline motors will work well with blends of 10% ethanol and also used as a solvent in industries. The ethanol produced from glucose and glucose extract from molasses with the help of yeast. The alcohol from fermentation is 8-10% and distillate it again and again to produce absolute alcohol. This is continuous and environment friendly process. Ethanol production have great impact on economy which reduced the import index of Ethanol. Equipment sizing for solutions is carried out and both operating and capital cost are used. The sensitive and significant parameters used to gain the product which is more efficient. The revenue generated per annum of product also identified.

Feasibility study and process optimization of citric acid production plant in KPK, using sugarcane molasses

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Abstract: Citric acid is one of the most lucrative weak organic acids produced using bioprocesses. One of the most common methods is the microbial fermentation of sugarcane molasses using bio-culture, Aspergillus Niger. Due to its multiple industrial applications, citric acid is in high demand all over the world. The use of citric acid in Pakistan is also rapidly growing but lack of indigenous production, demand is fulfilled through import from other countries, which costs more money and time. There is currently no active citric acid plant that can make use of the widely available raw material i.e. sugarcane molasses. Sugarcane molasses is largely produced in the province of KPK, Pakistan, without being utilized for industrial purposes. This study presents a feasibility study for the installation and process optimization of anhydrous citric acid plant in the feasible location of KPK Pakistan to meet the local industrial needs. Current study also involves the selection of a suitable and practical production unit consists layout of the chosen citric acid plant for a capacity of 100 metric tons per year, cost estimation, and the challenges during the project. The production of citric acid will help to resolve the waste disposal problem as well faced by sugar mills while also reducing the industry's reliance on other citric acid producers. As a result, the industry would be benefitted ecologically and economically.

Keyword: Feasibility, Citric acid, Molasses, Fermentation, Medicine.

Process development for production of bioethanol from lignocellulosic kitchen waste

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Abstract: Kitchen waste can be used as an effective renewable energy source as it is mainly composed of starch, carbohydrates, proteins, and organic acids, which can be used to produce biofuels through different approaches. In this study, a process was developed to produce bioethanol from lignocellulosic kitchen waste via enzymes produced by thermostable bacterium Thermobifida fusca and Saccharomyces cerevisiae in one pot. Pretreated kitchen waste was delignified by dilute acid and the filtrate of acid delignified kitchen waste was also investigated to observe the amount of total sugar and reducing sugar. The results showed that kitchen waste was best delignified at 1.5 % H2SO4 concentration for 90 min and 121 oC with 74 % delignification and 91 % cellulose recovery. At the same time, the conditions for the optimal growth of Thermobifida fusca in hagerdal media and time course of enzymes production required for saccharification by Thermobifida fusca was optimized. The concentration of reducing sugars was determined by DNS method and the concentration of total proteins was determined by Bradford method at different steps of whole process. The optimal temperature for the growth of Thermobifida fusca was found to be 50 oC and optimal pH of 6.0 in hagerdal media. In addition, the time course for the maximum production of both cellulases and xylanases was found to be 72 h at optimized conditions. These enzymes were used for the hydrolysis of treated kitchen waste into fermentable sugars and resulting hydrolysate was subjected to fermentation for ethanol production by Saccharomyces cerevisiae. Maximum saccharification of treated kitchen waste was found after 72 h of hydrolysis when 3% substrate concentration was used. The refractive index of ethanol produced in our laboratory was found to be 1.35, which is comparable with known refractive index of commercial ethanol.

Prediction and optimization of process parameters for biomass demineralization using RSM and ANN

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Abstract: Biomass is still considered an emerging sector for energy generation, however, its application in energy generation processes faces many technical challenges such as slagging, corrosion, and fouling on the heat transfer surface. These challenges present risks to the safe operation of biomass conversion processes and raise the maintenance cost of the operation. The demineralization process can address these issues by reducing the ash forming components in the biomass and making it a more valuable and efficient fuel. In the present work, demineralization of biomass was performed by treating rice husk with sulphuric acid at different temperatures (50-80 °C), time (30-100 min), and acid concentration (5-10 w/v%) while the responses are moisture content, volatile matter, ash content, fix carbon and hemicellulose. The optimization of these process variables was carried out using response surface methodology (RSM) and artificial neural network (ANN). The optimized values of process variables obtained from the models were 72.449 °C, 70.506 min, and an acid concentration of 8.156 w/v%. The acid treatment also improved the fuel properties of rice husk as heating value, fixed carbon, and volatile matter and resulted in approximately 40% ash reduction. The models obtained from RSM and ANN were also analyzed statistically using root mean square error, coefficient of regression, and absolute error, and it was concluded that the performance of both the models is satisfactory, but ANN provided lower error values than the RSM.

Food and Pharmaceutical

Kinetic study and application of artificial neural network (ANN) model to predict the degradation behavior of dairy manure

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Abstract: This study examines dried cattle dung originated from different breeds such as cow (CD), buffalo (BD), and a blend of CD and BD (CBD). Thermogravimetric analysis (TGA) data obtained in two different atmospheres were trained in Artificial Neural Network (ANN). The TGA data under inert atmosphere represents the thermal degradation behavior for pyrolysis, whereas the degradation in air atmosphere demonstrates combustion process. The samples were heated from ambient temperature to 800 °C for either atmosphere, at different heating rates: 20, 40, 60 and 80 °C/min. The heating rate and experimental temperature were taken as input parameters of ANN models and sample mass as output parameter. The obtained optimal models of ANN were able to predict the mass loss of samples at new heating rates (non-performed) within the specific range, with the correlation coefficient of 0.99999. The reproducibility of the ANN model was also analyzed. In addition to it, a linearized multi-stage kinetic model has been employed to study the kinetics during pyrolysis and combustion of candidate samples. The kinetic model accounts the initial sample weight (Wo) an essential consideration. The multiple stages of decomposition were determined based on the absolute local minimum values of conversion derivative (dα`/dt), obtained from DTG curves, which resulted in four decomposition stages during pyrolysis and three decomposition stages during combustion. The kinetic parameters, such as activation energy (Ea), pre-exponential factor (A) and reaction order (n), were computed for each stage. The Ea for pyrolysis at given heating rates (20 to 80 ^{o}C/min) varied between 19.57 to 64.47 kJ/mol, 60.19 to 87.08 kJ/mol, 197 to 237 kJ/mol and 20.47 to 28.83 kJ/mol for stage 1, 2, 3 and 4 respectively, with corresponding A (8.41E+02 to 3.31E+18 min-1) and n (0 to 3). Whereas, for combustion Ea fluctuated between 21.41 to 48.28 kJ/mol, 114 to 323.86 kJ/mol and 31.02 to 154.48 kJ/mol for stage 1, 2, and 3 respectively with A values of 1.20E+03 to 3.57E+30 min-1 and n, 0.6 to 3.

Keywords: Artificial neural network (ANN), Dairy manure, Multistage analysis, TGA

Synergic removal of CO_2 and NO using chemically modified activated Carbon prepared from food waste and scrap Tire

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Abstract: Globally, generation of food and tire waste (a significant portion of solid waste) is increasing because of population growth and economic development. In this study, a mixture of food and tire waste was pyrolyzed in the flow tube furnace to form biochar. Afterwards, it was chemically activated using ammonium iron sulfate (NH4)2Fe(SO4)2.6H2O at different activation ratios and activation temperatures of 1.0:0.5, 1.0:1.0, 1.0:1.5, and 1.0:2.0 and 500℃, 600℃, 700℃, 800℃, and 900℃ to produce chemically activated carbons. These samples of activated carbons produced were then evaluated to adsorb NO and CO2 gases at ambient temperature and pressure (25±2℃ & 1 atm) for both individual adsorption of gases and coal-based flue gas. This study investigated that maximum removal efficiency of NO and CO2 was found to be 99% and 98%, respectively at the optimum activation and temperature of 500℃ after 120 min. The surface morphology of the optimized activated carbon was studied using Scanning Electron Microscope (SEM) which showed highly porous structure. The optimized activated carbon exhibited a surface area of 1011 mg using Brunauer-Emmett-Teller (BET) analysis. Fourier transform infrared spectroscopy (FTIR) confirmed the presence of additional chemical groups such as -OH, -NH, etc., which might be activaly involved in the adsorption of NO and CO2 from flue gas. This study provides the potential that chemically modified activated carbon based on food and tire waste was suitable to remove CO2 and NO gases emitted from coal combustion.

Keywords: Solid waste, flue gas, coal combustion, adsorption, activated carbon.

Fabrication and characterization of stimuli-responsive hydrogels for drug release applications

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Abstract: The main focus of this research is on the fabrication of stimuli responsive hydrogels along with characteristics to regulate its function for controlled drug delivery. Natural and synthetic polymers were employed like pectin, chitosan and PVA blended with 3-aminopropyl(diethoxy) methylsilane to fabricate hydrogels through dissolution casting technique. Swelling investigation was done in deionized water, electrolyte and buffer solutions. FTIR and TGA were conducted to confirm functional groups, covalent and hydrogen bonding and thermal stability of prepared hydrogels. Gel fraction, contact angle measurement and porosity were also carried out to investigate crosslinking density, hydrophilicity and percent porosity of hydrogels. Biodegradation, cytotoxic nature and antimicrobial characteristics were determined using in vitro analysis. Finally accumulative ceftriaxone release was observed to be release in 180 min in phosphate buffer saline solution at 37 °C. The above results recommend these hydrogels to be use in control drug release applications.

Materials and Nanotechnologies

Multicomponent dyes adsorption onto adsorbent derived from plant waste: A Parametric Analysis

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Abstract: In the present research synthesis of "Ammonia Functionalized Carbon" was done by the reaction of "Oil Fly Ash" with the mixture of ammonia solution and phosphoric acid. The crystalline structure and phases of fly ash in raw form and after activation were determined by X-ray diffraction Spectrometry (XRD). Thermal properties were analyzed by Thermo-Gravimetric Analysis (TGA) and to study the potential of charged particles the technique of Zeta-Potential was applied. Main concern was the cheap and effective adsorption of "Methylene Blue & Rhodamine-6G) simultaneously from the wastewater. For this purpose, operational parameters pH, initial concentration of dyes, adsorbent dosage, and temperature effect for the removal of dyes were observed. After the analysis of uptake capacity and removal efficiency, optimized adsorbent dosage suggested for the process was 0.4g. Moreover, the nonlinear isothermal and kinetics model along with thermodynamic properties were highlighted and discussed. Single dye adsorption results were good as compared to the binary adsorption. For the binary dyes' solution, both dyes affect each other and the attraction among them decreases the adsorption ability of the AFC. Where it also can be observed that MB was more attractive towards the AFC and gives more adsorption regardless of the single and binary solution factor. Results showed that the most appropriate kinetic model for the process was "fractional order" with minimum error of 0.003 and best depiction of the single and binary adsorption with maximum R^2= 0.994 was through "Extended Langmuir Model". Thermodynamic model generated results conclude that involved single and binary phsyisorption process were spontaneous and endothermic.

Keywords: Binary Adsorption, Oil Fly Ash**,** Wastewater, Pollutant Dyes, Parametric optimization.

Titanium and Zirconium based metal organic framework (MOF) for pollutant gas purification

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Abstract: Recently, an outstanding nano material was invented called Metal-Organic-Framework that represents a new class of super-adsorbent. These structures are hybrid, porous, and multifunctional materials composed of metal clusters bonded with organic linkers. Such nano particulates are preferred over metal oxides, zeolites, and activated carbons on account of extensive surface area (mostly varying from 1,000 to 10,000 m^2/g), distinct pore structure, and tunable attributes. Moreover, newly synthesized MOFs manifested more thermal and chemical stability in comparison to traditional adsorbents. In this research, pristine (Zirconium, Titanium) and mixed metal (Zr/Ti) MOFs are synthesized by using solvothermal method and are studied for the adsorption of Sulfur Dioxide gas at ambient conditions. The NH_2-BDC linker is used in the synthesis of these MOFs. The relative adsorption capacities of the synthesized MOFs are greatly influenced by the variation in Zr to Ti contents. Also, the variation in Metal to Linker ratios (1:1 and 3:1) represented the considerable change in the uptake capacities for a particular gas. For the SO_2 gas, the adsorption capacities of MOFs (Metal to linker ratio, 3:1) with pure Zirconium and Titanium metals (Z100, T100) are calculated to 0.389 mmol/g and 0.452 mmol/g respectively, whereas the MOF with 70% Zr and 30% Ti (Z70T30) is computed to 0.699 mmol/g. However, the highest breakthrough capacity reported in this study is 0.962 mmol/g by using the MOF comprising of 30% Zr and 70%Ti (Z30T70). This class of MOF is dominant due to the thermal stability as compared to others which is verified by TGA (Thermo Gravimetric Analysis). The presence of required bonds in the MOF structures are identified by FTIR (Fourier Transform Infrared Spectroscopy). PXRD (Powdered X-ray Diffraction) technique is used to confirm the crystal structure. For the particular surface area in m^2/g, BET (Brunauer-Emmett-Teller) approach is used. The morphology of the nano crystals is examined by means of the SEM (Scanning Electron Microscopy).

Keywords: Metal organic framework, Sulfur dioxide, Pollution control, Adsorption, Breakthrough capacity.

Construction of Zn-based 3D-dimensional MOF via sequential insertion technique, accompanied by SC-SC transformation

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Abstract: Metal-organic frameworks are a fascinating class of porous functional materials assembled by combining metal nodes and organic linkers with diverse applications. These are generally synthesized by one-pot solvothermal reactions. This technique is associated with some disadvantages when various linkers are involved such as linker stability, linker solubility, formation of other domains and competition between the linkers. Recently, more valid strategies like post synthetic modification (PSM) of MOFs have proved to be effective in this case. In the present study replacement of structure building linker and sequential insertion technique has been exploited in order to convert a two-dimensional MOF (BUT-25) to three dimensional MOFs (BUT-26, 27) with distinct topologies. For the first time bent/angular linker was used instead of linear linker for example bipyridine. The sequentially inserted linkers were dicarboxylates (2,5-thiophenedicarboxylic acid and isopthathalic acid). The different angles between the arms of carboxylates may be the reason for two different and distinct topologies. All the MOFs were characterized by SC-XRD to elucidate their structures. The as-synthesized pxrd patterns matched well with simulated one. Further the efficiency of BUT-25 was checked for the detection of Fe^{3+} and $Cr_2O_7^{2-}$ ions in water. BUT-25 proved to be highly sensitive and selective towards these ions and also act as a colorimetric sensor.

Design and Synthesis of 2-D Cu-MOF, their structural diversity and applications

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Abstract: Recently, enormous research work has been carried out on Metal-Organic Frameworks due to their fascinating promising applications, but insufficient chemical stability prevents some practical applications, where the stability is very important for real-life environment. For the MOF stability, the metal-ligand coordination stability is pre-condition along with the orientations and configurations of ligand. It is believed that the rigid carboxy ligand provide stability to the framework. In this work we synthesized Cu-Fdc by solvothermal method and characterized by single-crystal X-ray diffraction (SXRD), powder X-ray diffraction (PXRD) and Brunauer-Emmett-Teller (BRT). More interestingly MOF can function as sensor and can detect traces of $Cr_2O_7^{2-}$ ions in water with high sensitivity and good selectivity. The detection limit (LOD) towards $Cr_2O_7^{2-}$ ions were calculated to be 0.37 µM. The effective fluorescence quenching phenomenon is credited to electron transfer between these ions and fdc^- ligand of the MOF. These LOD values are lower than the permissible values of these ions in drinking water permitted by EPA (US). In addition, the Cu-MOF showing good stability and exhibiting BET surface area 300 m^2/g. It is recommended that the 2-D Cu-MOF may have some good applications in the sensing of water-based metal anions.

Keywords: Cu-MOF, Furan-dicarboxylic acid, sensing, $Cr_2O_7^{2-}$ ions.

Synthesis and Performance of La-doped TiO_2 Nanocomposites for supercapacitors

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Abstract: Energy availability from the last decades has brought transformations in human life. Not only many of the energy resources have been ascertained, in addition to that diversification from fossil fuels to nuclear and other renewable sources has also been brought up. The world is observing large-scale novelty at energy production and consumption levels. The World needs sustainable and clean energy production as well storage methods. For the full replacement of fossil fuels, a storage system should be renovated to store the surplus amount of energy that can provide output at the instant. Researchers have reported the supercapacitors as the best substitute.

In the current research work, we have synthesized rare-earth-doped graphene-based nanocomposites containing TiO_2. TiO_2 was selected because it possesses remarkable electronic, dielectric, and physical properties. The hydrothermal method was adopted for the synthesis of composite. Graphene-based TiO_2 nanocomposites were synthesized with different concentrations of 0.5wt%, 1wt %, 2wt%, and 4wt% lanthanum. The synthesis of nanocomposites was confirmed through XRD analysis. The synthesized nanocomposites were also analyzed through UV-Vis and FT-IR techniques, and SEM. The synthesized nanocomposites were studied for their application in supercapacitors, through electrochemical testing including cyclic voltammetry, electrochemical impedance spectroscopy, and galvanostatic charge-discharge. 0.5wt% La-TiO_2 /RGO, 1wt% La-TiO_2 /RGO, 2wt% La-TiO_2 /RGO, and 4wt% La-TiO_2 /RGO exhibited capacitance of 95.12 F/g, 97.72 F/g, 100 F/g, 117 F/g, and 153.31 F/g respectively at 10mV/s.

Mineralogical Investigation and Exploration of the Mineral Potential Areas of Chitral, Pakistan

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Abstract: Mineralogical investigation is essential to determineminerals' constituents and nature in the ore for selecting the appropriate mineral processing technique. This paper presents the results of mineralogical analyses of the representative samples from mineral potential areas of Chitral, KPK, Pakistan in order to assess their composition and formation for valuable input in selecting a suitable processing technique. The samples ores were analysed using thin section study and x-ray diffraction (XRD) analysis, to comprehensively investigate constituents % age and type in selected samples. Mineralogical analysis of the samples revealed that the average %age of the copper contents is 10.31%, Iron 11.87%, silver 0.122%, gold 0.11 ppm and rare earths elements are in the range of 24 to 0.92 ppm. Investigation showed that mineral has high-grade copper, gold, silver iron with the anomalous amount of lead, zinc and traces of alumina, calcium oxide, magnesium oxide, nickel, and rare earths elements. Close examination of polished surface and thin sections study of ore samples confirmed that the deposit's main mineral is chalcopyrite $CuFeS_2$ with associated gold and silver while chief gangue minerals are andradite garnet $Ca_3Fe_2(SiO_4)_3$and Sphalerite (Zn,Fe)S. In order to further investigate the said mineralization for mineral potential, deposit extent, geological variation, and to study its economic potential, proper exploration operations are prerequisite by carrying out deep core drilling in the deposit and to carry out the characteristics study of the core samples.

Keywords: Precious Metals, Mineralization, Chalcopyrite, Andradite Garnet,Core Drilling.

Safety, Health, and Environment

Controlling Pollution in Hydroprocessing Units of Oil Refinery

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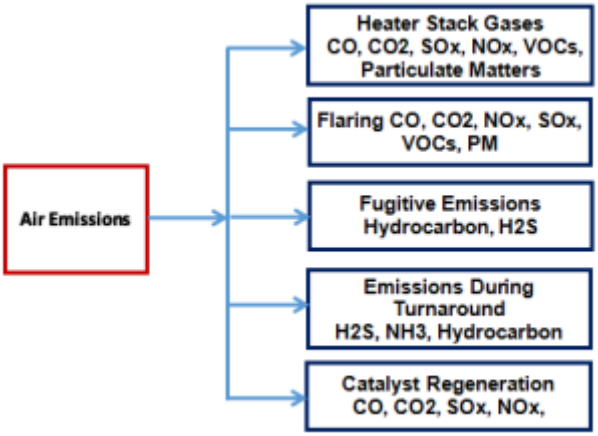
Abstract: The Hydrotreating process mainly removes Sulfur from Naphtha, Kerosene, and Diesel to produce environment-friendly petroleum products. On the other hand, during the operation of hydrotreating plants, numerous pollutants are produced which can be minimized by applying the best operational and engineering controls. Moreover, due to stringent environmental regulations, air emissions, effluent, and solid waste control are becoming challenging for refineries. These pollution problems should be taken as an opportunity to increase profits by reducing, re-using and producing valuable products from pollution products. In this article, I have emphasized predominantly operational controls and some engineering controls.

1) Emissions To Air: Air emissions from hydrotreating plants may arise from fired heater flue gases, flaring, fugitive emissions, catalyst regeneration, maintenance activities, etc.



a. **Fired Heater** is the major source of emissions CO, CO_2, NOXs, SOXs, Volatile Organic Compounds, particulate matter, etc.
   These pollutants can be minimized by improving heater efficiency, use of only oxygen for combustion, low sulfur treated fuel, utilization of ultra-low NOx burners, preheated fuel and oxygen etc.

   CO_2 from the flue gases can also be recovered using the Amine treatment method. CO_2 can be liquefied and sold due to its various industrial uses.

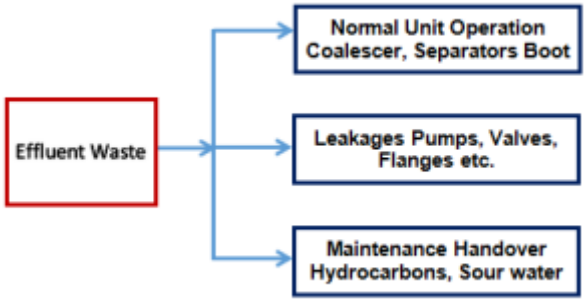
b. **Flaring:** In an oil refinery, flaring is required for burning off purge gases and other releases like an emergency, pressure safety valves, startups, and shutdowns.

   The highly suggested solution is to install a flare gas recovery system in the flare header of an oil refinery. This will not only save the environment but also save millions of dollars of gases from the refinery.

c. **Fugitive Emissions or leakages**; Emissions of gases or vapours due to leakages from pump seals, flanges, valves, piping, sampling points, etc. These can be minimized by monitoring, identifying, auditing, and rectifying the leakages.

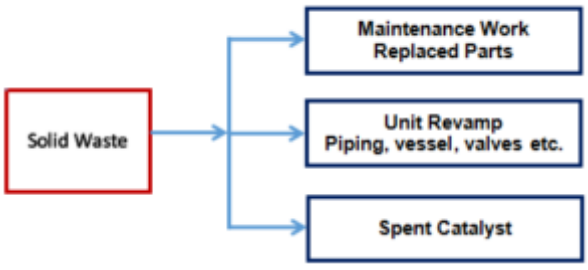
d. **In Situ Catalyst Regeneration:** In catalyst regeneration, Carbon and Sulfur accumulated on the catalyst are burned off. During this process, Coke, SO_2, CO, CO_2, particulate matter, and VOC (volatile organic compounds) are produced. The gases should be treated before discharging into the atmosphere. It is preferred to perform ex-situ catalyst regeneration.

2) Effluent Waste is generated from the normal unit operation, process upsets, maintenance activities, rainwater, spillage, leaks, etc. It is better to minimize the wastewater production or effluent treatment plant that must be efficient to treat and reuse the wastewater and recycle the value streams. The hydrotreating unit generates a flow of wastewater of 30~50 litres per ton of Diesel processed. The wastewater contains Sulphur compounds, NH3, hydrocarbons, suspended solids, etc. from spillage leaks.



3) Solid Wastes: Sources of solid wastes in hydroprocessing units are;

- Mechanical wastes like old equipment, valves, or pipes produced during the replacement of the revamping of the unit.
- Waste generated from maintenance activities like damaged parts or replacement of disposable parts like coalescing elements, filter cartridges, etc.
- Semi-solid sludge is normally removed from the process vessels during maintenance work in an annual turnaround.
- Metals particles due to corrosion in the process may result in the production of tons of solid in a year. Corrosion waste is collected at the reactor catalyst and high-pressure separator.
- Spent catalysts generated 50~200 MT/year depending upon the plant capacity. Spent catalysts may contain molybdenum, nickel, cobalt, platinum, palladium, vanadium iron, copper and silica, or alumina.



Novel and facile synthesis of Graphitic Carbon Nitride and Tungsten Oxide nanocomposites photocatalyst for the effective degradation of Methylene Blue

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Abstract: The quantity of organic contaminants in industrial wastewater is a critical worrying concern for aquatic life that can be hazardous to health, making natural water unfit for drinking. Synthetic colors are present in wastewater from the tannery and textile sectors, which are difficult to remove from water sources. Dye-containing wastewater is toxic to humans and aquatic life, as well as being carcinogenic and mutagenic in nature. As a result, it's critical to remove dyes from wastewater. In our research work Graphitic carbon nitride (g-C_3N_4) based Photocatalysts were prepared which works in the irradiation of light for the degradation of organic pollutants including Methylene Blue. Graphitic Carbon nitride nano-sheets Composites were made with the Tungsten Oxide nano particles (WO_3) in different percentages (5 percent, 10%, 15%, and 20%). Methylene Blue was degraded using the photocatalysts. UV spectroscopy was used to evaluate the photocatalytic activity of the prepared catalyst for the degradation of methylene blue dye under visible light (Xenon light). X-ray Diffraction, UV-vis DRS, and Photoluminescence (PL) intensity were used to characterize the synthesized catalysts. The PL intensity indicates that the recombination rate of g-C_3N_4 doped with tungsten oxide nano particles is reduced. For nanocomposite, the band gap of g-C_3N_4 was reduced from 2.79 eV to 2.69 eV. The tungsten oxide doped graphitic carbon nitride WO_3/g-C_3N_4 (20 percent) photo catalyst degraded methylene blue dye most effectively.

Keywords: Photocatalyst, Graphitic Carbon Nitride(g-C_3N_4), Tungsten Oxide (WO_3) Nano Particles, Methylene Blue.

Response Surface Methodology for optimization of operational parameters for electrochemical disinfection of drinking water

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Abstract: Natural water has been contaminated with microorganisms and pollutants due to several climate changes and human activities. Disinfection is a critical issue because water borne pathogens can lead to various fatal diseases like cholera, dysentery and typhoid. The electrochemical disinfection (ECD) is a green technology, identified as cost effective, chemical free and environment friendly alternative for disinfection purposes. In current study, for disinfection of canal water stainless steel 316 grade electrodes were used in a batch type electrochemical reactor with a volume of 4L. The experiments were designed using box-benken design in response surface methodology. Three operational variables were selected, namely current density (0.25-2.5 mA/cm^2), inter-electrode spacing (0.5-2.5 cm) and treatment time (0-10 min) to optimize the disinfection efficiency using response surface methodology. Disinfection efficiency was chosen as response variable while current density, operational time and inter electrode spacing were selected as independent variables. RSM optimization show that the maximum, 93.5 % disinfection efficiency was achieved at current density 1.38 mA/cm^2, inter-electrode spacing 1.5 cm and treatment time 5.5 min. Furthermore, results revealed that the current density and treatment time positively effects the disinfection efficiency. However, a significant behavior was observed for inter-electrode spacing. Increasing the inter-electrode spacing reduces the disinfection efficiency. At optimum values of process variables the energy consumption and operational cost for disinfecting $1m^3$ of water was 0.256 kWh 6.4 PKR respectively.

Synthesis of Composite Membranes for Reverse Osmosis Applications

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Abstract: With a growing world population and human activities, pure water availability is becoming main environmental challenge. Membrane based technologies are best solution for such a problem. In this study thin film composite membranes will be synthesized and used to address the problem of water purification through reverse osmosis technique. A thin film composite membrane will be synthesized in the form of film from two or more layered materials that will be anisotropic in nature and have high salt rejection, good mechanical strength, and high filtration rate. Polymeric membranes e.g., cellulose acetate membranes will be combined with an inorganic material e.g., GO, TiO_2 etc. to get a composite membrane. For this electro-spinning method will be used. Synthesized membrane will be characterized through SEM, TGA, DSC, and FTIR to analyze membrane structures and properties to find out most efficient synthesized membrane.

Sodium Alginate Based Nanocomposite Membranes for Oil-Water Separation from Wastewater

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Abstract: In the current situation, wastes from industries, notably the petroleum sector, at any stage from drilling through transportation, are important environmental issues. In this study hydrophilic graphene oxide (GO) and Zinc oxide nanoparticles (ZnO NPs) were synthesized and employed as a filler in the fabrication of efficient and robust Sodium Alginate (SA) nanocomposite membranes for oil-water separation using pressure driven filtration approach. These membranes prepared by solution casting and crosslinking method were found to be extremely hydrophilic, with increased porosity, pure water flux (PWF) and mechanical strength. The antifouling test of the nanocomposite membranes revealed significant improvements over the pristine SA membranes without the need for alkaline or acidic cleaning. The composite membranes' morphology, structure, mechanical strength, thermal stability, and wettability were studied using Scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), X-ray diffractometry (XRD), tensile testing, Thermogravimetric analysis (TGA) and water contact angle measurement, respectively. Separation efficiency, pure water flux, and flux recovery ratio (%FRR) were all investigated. The findings reveal that incorporation of 1.5 weight percent GO and 0.1 weight percent ZnO NPs to the SA matrix resulted in increased oil removal efficiency along with prominent advantages of cost effectiveness and environmental friendliness.

Keywords: Sodium alginate; Graphene oxide; Zinc oxide NPs; Nanocomposite membranes; Mechanical strength; Oil-water separation.

Relationship Between Air Quality Index and Meteorological Parameter Among the Major Cities of Pakistan

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Abstract: The aim of present study was to compare the ambient air quality among major cities of Pakistan, which includes Karachi, Lahore, Faisalabad, Bahawalpur, Gujranwala, Rawalpindi and Islamabad and its relationship with meteorological parameters. Exposure to fine particles may cause short-term health effects such as eye, nose, throat and lung irritation, coughing, sneezing, mucus dripping and shortness of breath. Meteorological parameters and air quality index (+IQAir) data for selected major urban cities was obtained from two sites namely time and date and +IQAir site for the year 2020. Parameters such as temperature.

Status of greenhouse gases (CO_2, CFCs, CH_4, N_2O, O_3) in Pakistan, associated health and environmental effects, and future directions for their mitigation

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Abstract: Pakistan is a geo-politically significant country in South Asia, ranking 5th in the world with respect to population. It shares its borders with India, China, Iran and Afghanistan. The country has four provinces, FATA and disputed territory of Kashmir. Pakistan is an over-populated country giving rise to various developmental and management issues like capital reduction, unemployment, child development, and urbanization. The reasons of overpopulation can be high fertility rate, illiteracy, lack of birth control, socio-religious factors, rural and early age marriages, and urbanization. Pakistan holds a significant position with respect to climate change and environmental conservation. Pakistan's climate is of continental type, arid and semi-arid, which is characterized by extreme variations in temperature, both seasonally and daily, because it is located on a great landmass north of the Tropic of Cancer. The climate varies from arid to semiarid where three-fourth part of the country receives rainfall of less than 250 millimeters (mm) annually, except in the southern slopes of Himalaya and the sub mountain region in the northern segment of the country, where annual rainfall ranges from 760 mm to 2,000 mm. According to the national GHG inventory of Pakistan for the year 2011–2012, its total GHG emissions was at 369 million tons of carbon dioxide equivalent with 45.9% share of energy, 44.8% share of agriculture and livestock sector, 3.9% share of industrial processes, and 2.6% share of land use change for forestry sectors. Carbon dioxide (CO_2) is most significant greenhouse gas as it contributes more than 70 % of atmospheric concentrations. In the last few decades, emissions of CO_2 have increased rapidly. Combustion of fossil fuels and land-use conversion is the primary source of CO_2 emissions. Lahore, the capital of Punjab has been ranked at the first place for being the most polluted city in the world during the winter months and observance of smog in the region. Methane is an important greenhouse gas and a major environmental pollutant, second only to CO_2 in its contribution to potential global warming. The major GHGs include ozone (O_3), and N_2O, which have major sources in energy sector, waste sector, industrial sector, and agricultural sector. Greenhouse Gases also have severe impacts on the human health, which have been described in detail in this paper. These health impacts affect the people of different areas in different manner due to the variations in concentration and climatic conditions. United Nations has been working to control the impacts of climate change my making different legislations which date back to 3 to 4 decades including Montreal Protocol (1987), Kyoto Protocol (1997), Doha Amendment (2012), and Paris Agreement (2015). Also, Sustainable Development Goals (2030) have been designed to achieve climate stable world by no later than 2050.

Turnaround Safety Considerations

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Abstract: Turnaround (abbreviated as TAR, TA, or ATA) is a planned event wherein an entire process of a plant (refinery, petrochemical plant fertilizers plant, etc.) is taken off-stream for a long duration (more than a month) to perform equipment overhauling, cleaning, inspection, maintenance, replacement, modifications, piping work, etc. Turnarounds are non-routine, troublesome, complex, and potentially more hazardous than normal plant operations. The situation becomes more complex and hazardous when revamp of the unit is also involved along with a turnaround. Moreover, a short shutdown for partial maintenance of equipment is also a big safety risk because some sections of the unit remain pressurized with process chemicals. Safety must be the top priority in every step of shutdown or turnaround otherwise accidents may happen.

These are selected turnaround safety topics and can be converted into turnaround safety presentations. Further, this can be a good material for turn-around safety toolbox talk. Mainly, these are written for oil refinery safety but can also be followed in the petrochemicals, chemicals, fertilizer processing plants, and for oil and gas to safely conduct the shutdowns. Although these turnaround safety guidelines are written for long shutdowns but are equally applicable for the short shutdown of the unit for partial maintenance and repair of equipment.

Safety Considerations During a Turnaround or Shutdown:

1. Unit Shut down for Maintenance Handover in Turnaround
2. Steam Out of Process Piping for cleaning
3. Water Flushing for process piping cleaning
4. Nitrogen Purging meaning
5. Equipment Handover for Blinding and Maintenance
6. Chemical cleaning
7. Hot works hazards and control measures
8. Safety precautions for couplings and fittings
9. Flexible and pressurized hoses safety
10. Catalyst Unloading and Loading Safety Hazards
11. Electrical Hazards
12. Work at height
13. Pyrophoric Materials Safety
14. SIMOPS (Simultaneous Operations)
15. Confined Space Safety
16. Poor Housekeeping
17. Communication Hazards
18. Austenitic Stainless-Steel Protection
19. Extensive Working Hours

The Implementation of Membrane Technology Processes to Resolve Water Problems in Pakistan

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Abstract: Water pollution has been increasing globally due to increase in industrialization and population [1]. Polluted water and inadequate solid waste management, both are a threat for human health and green environment. It is sad to say, however, at a government level and publicly, there is no serious efforts taken to treat the polluted water in developing countries, including Pakistan; consequently, water-borne diseases are left to spread without any interference. Due to lack of wastewater-treatment facilities, the natural environment and public health continues to suffer, especially those areas which are adjoining industrial sites [2].

Pakistan, a country struggling to undergo development, is currently facing a huge population explosion and its populace is expected to jump from 170 million to 221 million at the end of 2025. This enormous boom in population will naturally have an adverse effect on Pakistan's water consumption; especially for the industrial, domestic and the agricultural sector [3].

Quality of drinking water is a major concern in most areas of the country, not just a few big cities like Karachi; rural areas are negatively affected as well. In the South of Punjab, 20% of water sources are high in arsenic concentrations, resulting in skin disease and/or cancer being common in the region. Also, contamination and pollution by industrial waste or bacteria leads to major problems too. Therefore, there is a need for policies to be implemented to ensure water quality standards and to raise awareness about the significance of safe drinking water, especially where the health of the future generation is concerned [4].

In our research we have come across an inexpensive and effective method to separate constituents that are dissolved or suspended in a liquid via membrane filtration. The membrane consists of a bodily obstacle that prevents harmful components, based upon their chemical and/or physical properties from passing through, while allowing others to flow through easily.

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Venue

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Day – II | Friday – March 25, 2022

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