Supervisor: Prof. Arvind Kumar Sharma

Project Topic: Hydrodynamic and Mass Transfer Aspects of Multiphase Systems

Wastewater [liquid (L)] may be taken as a multicomponent mixture/solution of variable composition, having various species of chemical, biochemical and/or biological nature. Treating it means de-mixing/separation of these species via physical, chemical and/or biological methods which involve other phases [gas (G) and/or solid (s)].

Examples being: aerobic processes using air/O_2 [G-L systems]; adsorption using adsorbents [L-S systems]; anaerobic attached growth [G-L-S systems] and similarly other multicomponent-multiphase systems, of which single/binary-two phase systems are simplifications/subsets.

Flow pattern of wastewater [liquid (L)], through hydrodynamics, and de-mixing/separation of species via mass transfer are important and integral parts of wastewater treatment systems. Understanding these aspects helps us to improve these processes so that they become more efficient by becoming less material/energy intensive and hence more sustainable.

Our group is, presently, focusing on 2 such systems: multistage liquid-solid fluidized bed and reversed jet loop reactor, L-S and G-L systems respectively. These 2 experimental setups have been designed and constructed by our group. We are open to other systems as well. We respect both: experimental and theoretical/computational approaches for solving the problems along with a judicious blend of both depending upon the facilities present/created and one's natural orientation/inclination towards research.

Being specific for fluidized beds, Fluidized bed adsorber (FBA) is characterized by high degree of mixing and short residence time(s). Hence, the removal of pollutants using FBA may not be complete. For high removal of pollutants, the fluidized bed can be staged resulting in longer residence time. The multistage operation enhances the overall concentration gradient in the liquid phase and hence increases the mass transfer rate. The multistage FBA can be operated with the solids (adsorbents) either in batch mode or in continuous mode with solids flowing counter-currently to the liquid phase (wastewater).

For successful analysis, design and operation of fluidized bed adsorber, information on equilibrium, hydrodynamics and adsorption characteristics of the (liquid-solid) fluidized bed is required. Parameters for investigation include: mode of operation (single & multi-stage and adsorbents in batch & continuous modes), particle size, adsorbent loading, fluidization velocity, types & concentration of pollutants along with regeneration and reuse. Apart from systematic experimental studies, a judicious blend of fundamental insight will be incorporated via developing comprehensive model(s) and/or correlation(s) for understanding, describing and predicting the behavior of fluidized bed adsorber for the removal of different pollutants from wastewater.

Idea has been/is to take what we have/can learn(ed) elsewhere, to what we are/can do(ing).

More Details | pls visit: http://universe.bits-pilani.ac.in/pilani/arvinds/Research

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Supervisor: Dr. Bhanu Vardhan Reddy Kuncharam

Project Topic: Novel Mixed-Matrix Membranes for Separation of CO2 from Biogas and Natural gas
Broad Research Area: Membranes Separations, Gas Separation, Separation Processes

Background of Research:
Biomass such as agricultural waste, landfill, sewage, and industrial waste is abundantly available in India. Biomass can be converted into biogas – a mixture of methane, carbon dioxide, and other impurities – using anaerobic digestion. Biogas can be used as an energy source. The calorific value of the biogas mixture can be increased by the removal of Carbon Dioxide. Membrane systems can be used for the separation of carbon dioxide from biogas mixture. This project's primary focus is developing asymmetric composite mixed-matrix membranes for the removal of Carbon Dioxide from the Biogas mixture under harsh conditions.

Responsibilities/Expected Outcome from the student:
This project involves experimental work as well as developing mathematical models for membranes. The primary responsibilities of a student are as follows:

- Screen the suitability and compatibility of polymer and inorganic filler material for CO_2 and H_2S separation from CH_4 from the literature and using various theoretical tools.
- Prepare asymmetric composite mixed-matrix membranes
- Characterize the prepared membrane using SEM, FTIR, and XRD; characterize in terms of inorganic filler dispersion, and defects (if any), modify the technique until uniform dispersion, higher filler particle loading, and defect-free samples are achieved.
- Conduct experiments to test the performance of the prepared membrane for the selectivity and permeation of CO_2/CH_4 separation from raw biogas (with and without the presence of H_2S).
- Develop a mathematical model to predict the performance of the membrane for CO_2 removal from Biogas derived from various sources.

Selected Publications
- Neha J, Nirmal Kumar S, Priya T. S, B.V.R Kuncharam, "Synthesis And Characterization Of Mixed-Matrix Material Of Zirconium Based Metal-Organic Framework (MOF: UiO-66-NH2) And Poly(Ether-Urethane-Urea)", Materials Today: Proc.
- B.V.R Kuncharam, and A.G Dixon, "Multi-scale two-dimensional packed bed reactor model for industrial steam methane reforming", Fuel Processing Technology, 2020, 200, pp 106314.
- BVR Kuncharam, BA Wilhite, "Theoretical investigation of a water-gas-shift Catalytic membrane for diesel reformate purification", AIChE Journal, 2013, 59 (11), 4334- 4345.

Essential Qualifications:
- M.E./M.Tech. with at least 60% marks in Chemical Engineering
- Exceptional MSc Chemistry candidates may be considered

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Supervisor: Dr. Somak Chatterjee

Project Topic: Synthesis of thin film composite membranes for organic solvent nanofiltration

Broad Research Area: Material Science, Polymeric Science, Membrane Science and Water Filtration

Background of Research: In recent decades, organic solvent nanofiltration (OSN) with membranes has been very attractive due to its high separation efficiency and low equipment costs and energy consumption. Different materials have been explored for the manufacture of high-performance composite membranes. These include carbon nanotubes, graphene, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs), among others. MOFs are of great interest due to the exceptional properties of the design and functionalization of their pores, their high specific surface area and their easy synthesis, contributing to several membrane applications. These materials can successfully be impregnated with a suitable polymer to prepare thin film composite (TFC) membranes that can have high selectivity and productivity.TFC membranes comprise a non-woven support at the bottom, an intermediate layer with an asymmetric porous structure, and a selective ultrathin film at the top. One of the most commonly used porous supports are polyimides (PI) owing to their unique physicochemical properties such as their resistance to high temperatures, radiation and chemical attack, their good mechanical strength and their superior insulation properties. Usually, OSN membranes face challenges mainly in terms of the formation of defect-free skin layers with minimal thicknesses and of highly stable and selective operation. Thereby, this PhD topic is floated to ensure the applicability of different coating methods and materials to form defect free OSN membrane, which are mainly thin film composite types.

Requirements:
- ME/M.Tech in Chemical Engineering (Exceptional candidates having MSc degree in inorganic Chemistry will be considered) with at least 60% marks throughout the entire career
- Knowledge in synthesis of polymeric membranes, characterization, corresponding experimentation and mathematical computation
- Hardworking and good knowledge in english for technical paper writing
- Good lab ethics, technical and professional transparency

Selected Publications:

1. Biswal, L., & Chatterjee, S. (2022). Metal organic frameworks (MOFs) in aiding water purification from emerging and ionic contaminants. In *Development in Wastewater Treatment Research and Processes* (pp. 651-668). Elsevier.
2. Biswal, L., Goodwill, J. E., Janiak, C., & Chatterjee, S. (2021). Versatility, Cost Analysis, and Scale-up in Fluoride and Arsenic Removal Using Metal-organic Framework-based Adsorbents. *Separation & Purification Reviews*, 1-19.
3. Sarkar, I., Chatterjee, S., & Kumar, K. H. (2021). Synthesis of thin film nanocomposite membranes and their application in dye removal from wastewater. In *Membrane-Based Hybrid Processes for Wastewater Treatment* (pp. 367-383). Elsevier.
4. Chatterjee, S., Mukherjee, M., & De, S. (2020). Groundwater defluoridation and disinfection using carbonized bone meal impregnated polysulfone mixed matrix hollow-fiber membranes. *Journal of Water Process Engineering*, *33*, 101002.
5. Chatterjee, S., & De, S. (2014). Adsorptive removal of fluoride by activated alumina doped cellulose acetate phthalate (CAP) mixed matrix membrane. *Separation and purification technology*, *125*, 223-238.

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Supervisor: Dr. Krishna C. Etika

Project Topic: 3-D Printed Hybrid Polymer Nanocomposites for Stealth Applications

Broad Research Area: Advanced Materials, Nanotechnology, Polymer Nanocomposites

Background of Research: Fused deposition modeling (FDM) is a heat-assisted 3D printing process in which the molten polymer is extruded out of a nozzle, deposited onto a substrate, cooled down, and solidified . FDM generates multilayered, multifunctional structures as well as patterned structures with complex geometries. The multilayered patterned structure is a novel empowering technology that allows controlling the properties of each layer/section of the shield, and thus manipulate the shielding mechanisms, not possible in common molding techniques. Another significant advantage of 3D printing is the development of stealth shields with complex geometries, which is a critical need in advanced industries such as aerospace and defence. The technology of the 3D printed shields is in its infancy and the underlying science is an ongoing subject of investigation in the literature. To explore the realm of 3D printed shields we will employ a variety of strategically chosen conductive, magnetic and dielectric nanofillers. The ultimate outcome of this research would be to produce a fully biodegradable, mechanical robust, lightweight materials with greater than 20 dB microwave absorption loss.

Responsibilities/Expected Outcome from the student:
This project involves the 3D printing of pristine polymer and its nanocomposites to create radar absorbing materials with complex geometries. We will investigate the influence of different parameters, such as filler loading, electrical conductivity of the filament feedstock, number of layers, architecture of the scaffold, patterned structure, dispersion state of filler, on the final electrical, mechanical, and shielding properties of 3D printed samples.The primary objectives of the proposed research expected from the student are as follows:

1. **Task 1**: We will use the chemical technique to synthesize magnetic and dielectric nanoparticles of interest. The nanoparticles would be carefully selected based on their properties.
2. **Task 2**: We will develop and characterize biodegradable (Polylactic acid based) nanocomposite pellets and filaments by mixing various types of nanofillers from Task 1. The mixing will be performed at various loadings of nanofillers ranging from 0.1-5.0 wt%.
3. **Task 3:** We will compression mold the materials into various shapes and characterize them. The compression-molded samples will be used as a benchmark to evaluate the quality of nanofillers employed and the performance of the 3D printed samples.
4. **Task 4:** We will 3D print the developed pristine polymer filaments using the FDM technique and characterize the samples.
5. **Task 5:** We will 3D print the developed nanocomposite filaments using the FDM technique and characterize the samples.

Publications

https://scholar.google.com/citations?user=e4kYT2IAAAAJ&hl=en

Essential Qualifications:

- M.E./M.Tech. with at least 60% marks in Chemical/Materials/Nanotechnology
- M.Sc. Chemistry/Materials Science candidates with very good track record will also be considered

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Supervisor: Dr. P C Sande

Project Topic: CFD simulations to study, enhance and design industrial multi-phase operation.

Broad Research Area: CFD simulation

Background of Research: The field of computational science is affecting design, scale-up and improvement of industrial chemical engineering unit-operations. Fluidized beds in particular are widely employed, and are among the more complex unit operations owing to the variety of regimes that they display, such as: Homogeneous, bubbling, turbulent and slugging fluidization. These regimes emphatically affect reactor performance .They are ideal to be investigated by computational and simulation tools that have developed over the past decade such as: ANSYS Fluent, OpenFOAM, COSMOL etc.

Requirements:

1. Knowledge of basic fluid dynamics
2. C++ programming experience
3. Visual discernment of patterns/ pattern recognition
4. Adequate scientific writing skills

   For preference: Experience of CFD software or coding for numerical methods

Publications

- P.C. Sande, S. Ray, Fine Mesh Computational Fluid Dynamics Study on Gas-Fluidization of Geldart A Particles: Homogeneous to Bubbling Bed, Industrial & Engineering Chemistry Research, 55 (2016) 2623-2633.
- P.C. Sande, S. Ray, Mesh size effect on CFD simulation of gas-fluidized Geldart A particles, Powder Technology, 264 (2014) 43-53.

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Supervisor: Prof Suresh Gupta

Project title: Development of Eco-friendly microporous polymer-metal frameworks for pollutant adsorption

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