

"Department of Chemical Engineering, IIT Bombay.
Preference for TA, TAP and FA Ph.D Topics for Autumn, 2022-2023
You have to submit your preferences based on the following topics before 03/05/2022 in the google form shared in the departmental (Chemical Engineering) website
You should attend the online discussion session to know "How to fill the preference form on 30/04/2022

Timestamp	Type of the project (TAP, TAP or FA, FA)	Email Address	Name of the faculty	Title:	Objectives (4-5 lines):	Nature of the project (Experimental/Modeling/Theoretical):	Background required (e.g. Chemical Engg./Chemistry/Physics, Specific experimental expertise/Knowledge in coding,	Link to the additional information (Additional description, videos etc.) [Optional]
1(TA)		----	----	---	(Guide and topic will be decided after one semester based on the availability of the topics and positions with the faculty)	----		
2(Atq)	TAP or FA	amalani@iitb.ac.in	Ateeque Malani	Simulation studies of enhanced oil recovery using CO2 and steam	The crude oil in direct contact with mineral surface needs to be displaced using external medium (solvent + additives) in the secondary and tertiary phase of recovery. The mechanism of replacement is governed by the structural and energetic behaviour of interfacial system (solvent + additives + hydrocarbon oil) at the mineral surface. This project is aimed to study oil displacement capacity of CO2 and Steam using molecular simulations.	Theoretical/Computational	Chemical/Petroleum/Chemistry/Physics. Students with strong motivation for research, maths, chemical engg/chemistry and coding are encouraged to apply.	
3(Atq)	TAP or FA	amalani@iitb.ac.in	Ateeque Malani and Jhumpa Adhikari	Gas hydrate formation and inhibition: Thermodynamic and Molecular Simulation Study	During transport of crude oil and gas, often gas hydrates are formed in pipelines which creates flow assurance problem. Gas hydrates are found in deep reservoirs as well. For efficient transport of crude oil, prevention of gas hydrate formation is necessary. The project aim is to understand the thermodynamics and kinetics of gas hydrate formation and prevention using external chemicals.	Theoretical/Computational	BTech, MTech in Chemical/Mechanica/Petroleum and other related, MSc in Chemistry/Physics/Material Science	
4(DVK)	TAP or FA	khakhar@iitb.ac.in	Devang V. Khakhar, Partha S Goswami	Rheology and dynamics of dense, turbulent fluid-solid flows	Turbulent, dense fluid-particle flows are commonly encountered in engineering processes such as in air jet mills as well as terrestrial and extra-terrestrial phenomena, e.g., bedload sediment transport, movement of sand dunes, impingement of jets on planetary surfaces. High speed fluid flows on dense beds are complex in nature because of the coupling between the fluid and solid phases. The project aims to account for the effect of fluid phase fluctuations on the particles using LES (Large Eddy Simulation)/DNS (Direct numerical Simulations) and particle feedback force using particle resolved technique. Simulation results will be compared with the experimental observations of high speed particle image velocimetry. An important impact of the project will be to enhance the basic understanding of the dense gas-solid flows. The project will result in the development of a computer code for such systems, validated by experiments, as well as continuum two-fluid models, which can be utilized for the analysis and design of practical systems.	Includes both, experiments and modeling	Chemical Engg./Mechanical Engg./Physics	
5(AMS)	TAP or FA	amol.subhedhar@iitb.ac.in	Amol Subhedhar	Development of lattice Boltzmann model for two-phase flow with phase change and its application to drop evaporation problem:	Lattice Boltzmann is increasingly becoming the method of choice for the numerical solution of fluid dynamical equations. This method has an advantage in dealing with wetting and no-slip boundary conditions in complicated geometry. The project will focus on formulating a model for two-phase flow with phase change in one class of multi-component lattice Boltzmann method. The challenge here is to ensure that the emergent macroscopic solution of the lattice Boltzmann scheme is in line with the general kinematic condition at the fluid-fluid interface. A multi-scale analysis will be used to show the feasibility of the model. The project will have a programming component where an existing code (in c++) will be modified. This model will be applied to the drop evaporation problem, which involves high-density contrast and wetting boundary conditions.	Theoretical/Computational	Interest in algorithms, coding	
6(OM)	TAP or FA	ojumohan333@gmail.com	Ojus Mohan	Hydrogen generation via catalytic methane pyrolysis in molten media	Hydrogen has the potential to replace fossil fuels as a sustainable energy carrier in a variety of applications. However, conventional hydrogen production technologies (electrolysis, methane reforming reaction) are either costly (electrolysis) or emit CO/CO2 into the atmosphere (reforming reaction). Alternately, catalytic methane pyrolysis (CH4(g) → C(s) + 2H2(g)), enables the possibility to produce CO2-free hydrogen from natural gas. However, previous attempts to employ solid metal catalysts failed due to the catalytic deactivation caused by carbon formation on the surface and/or its diffusion into the bulk of the catalyst. Remarkably, the deactivation of the catalyst can be avoided by performing the reaction in molten medium (molten metals or molten salt) since the carbon floats on the melt surface. Additionally, if C-C coupling can be facilitated, we may fully eliminate carbon formation and obtain more valuable C2 products, along with hydrogen. The key objectives of the proposed computational study are to i) screen molten media for methane pyrolysis, ii) enhance the catalytic performance of molten media without compromising its stability, and iii) facilitate C-C coupling by dispersing metal catalysts into the molten media.	Theoretical/Computational	Chemical Engineering	
7(VG)	TAP or FA	venkatg@iitb.ac.in	Venkat Gundabala and Abhijit Majumder	Development of a microfluidic device to study Cancer-Associated Fibroblast (CAF) and Breast cancer tumor interactions in 3D	In this work, we propose to employ a microfluidics platform to develop a 3D core-shell breast tumor model in which tumor cells and CAFs will be cultured in close proximity. The student will use microfluidic techniques to generate cell encapsulated microparticles and microcapsules. Further, biological studies such as growth, migration, and chemo response of tumor cells in co-culture conditions will be conducted. The final findings from this study are expected to contribute towards expediting the efficient treatment of breast cancer which is affecting millions of women in India. The project will be co-supervised by Prof. Abhijit Majumder.	Experimental	Background required in Biotechnology/Biomedical engineering with good experience in experimental techniques such as cell culture, microscopy, and molecular biology.	
8(VG)	TAP or FA	venkatg@iitb.ac.in	Venkat Gundabala and Abhijit Majumder	Microfluidics based generation of microcapsules for breast cancer tumor studies	Breast cancer is the most common cancer in women in India and accounts for 14% of all cancers in women with high prevalence and mortality rate. However, one of the major hindrances in drug discovery as well as drug screening is unavailability of suitable model system to mimic true tumor microenvironment (TME). In this project, the student will design and fabricate microfluidics based devices to generate 3D particles and core-shell microcapsules to mimic TME. Using these 3D entities, studies on conversion of MSCs into CAFs and growth of tumor cells in the presence of CAFs will be performed. With its unique ability to precisely tune the sizes of the microcapsules, this microfluidics based approach will allow investigation of the effect of not only the morphology of the TME but also the size of the TME. The project will be co-supervised by Prof. Abhijit Majumder.	Experimental	Required background in Chemical engineering with good fundamentals and experience in experimental projects. Prior experience in microfluidics and exposure to biological projects is a plus.	

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9(RB)	TAP or FA	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	On the mechanism of nanoparticles in water disinfection: Using microfluidic devices to understand and design point of use systems	<p>Disinfection of water at point-of-use (POU) can remove microorganisms, providing clean and safe drinking water. Disinfection by metal nanoparticle (NP) impregnated activated carbon (AC) is proposed in this project. This will be done in a gravity-driven filter-column set-up, which would run without any power, ideal in a resource-constrained scenario.</p> <p>Understanding the interaction between NPs and bacterial cells is thus crucial to explain the device performance. The project aims to uncover such biotic-abiotic interactions by microfluidic experiments, involving bacterial cell-laden water being flown, over PDMS gel casted or 3D printed channels (with different patterned surfaces), mimicking the intergranular pore structure of AC.</p> <p>The optimum hybrid material in terms of NP size and surface number density of these particles, on different patterned carbon surfaces would be found, to be used for the gravity-driven POU system.</p> <p>Thus, for the first time, experiments based on microfluidic platforms will result in development of a new engineering design of a power-free water disinfection system.</p> <p>The work will be as part of a team of other students with interdisciplinary background, with ample scope to learn and innovate.</p> <p>The research involves: (i) either designing and conducting experiments with microfluidic devices, or (ii) engineering of water treatment systems.</p>	Experimental	(i) MTech/ME/BTech/BE in Chemical/Mechanical/Environmental/Materials Engg. or allied Engg. branches or (ii) MSc in Physics/Chemistry/Materials Sc. or allied basic science depts.	
10(RaD)	Only TAP	dasgupta.ratul@gmail.com	Ratul Dasgupta	Numerical simulations of wind over ocean waves - DNS and LES	This is a joint project between three IITs (Ropar, Chennai & Mumbai) funded by DST-SERB. The project involves Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) of wind generated ocean wave, their breaking and sea spray generation. An experimental facility for generation of wind driven waves is being setup at IIT Ropar and there will be opportunity to travel to Ropar and Madras for joint meetings and discussions and comparing simulation generated data against experiments. Apply to this project if you find computational fluid mechanics (CFD) interesting and also enjoy thinking of maths and physics problems.	Theoretical/Computational	B.E. in Mechanical, Aerospace or Chemical Engg., Physics (MSc) with interest in fluid dynamics	
11(BKS)	TAP or FA	bharat.k.suthar@iitb.ac.in	Bharatkumar Suthar	Enabling e-mobility through accurate measurement of nanoscale processes in li-ion battery	Accurate battery model is the key for designing a battery pack for e-mobility applications ensuring safe and efficient battery operations. While simplified battery models (equivalent circuit models) are desirable for control-relevant application, detailed electrochemical models which connect the dynamics at the nanoscale to the sub-mm scale (and larger) are needed for designing battery pack as well as coming up with its usage (charging/discharging) policy for long-lasting and safe battery operations. Tremendous engineering efforts at the nano-scale goes into designing battery materials that are safe and have a long life. While the general modeling frameworks incorporating the dynamics at the nano-scale are well established in literature they require a set of parameters to be accurately measured. This project relates to taking a commercial battery (where very little is known from the manufacturers), opening it up, and coming up with ways to measure as many parameters as possible. Such measurements will be electrochemical (transport properties of lithium/lithium ions in nanopores or nanoparticles), physical (size distribution, pore network, porosity, tortuosity, etc.), chemical (composition and distribution of elements in nanoparticles), thermal (heat conductivity) or electrical (resistances) in nature. Accurate measurement of such parameters will enable the development of an experimentally validated battery model of a commercial li-ion cell. Such models will be key to ensure safe and lasting battery operation as well as a detailed design of battery packs for various applications	Includes both, experiments and modeling	Chemical engineering (Transport phenomena, reaction engineering, numerical and computational methods) Both experimental and modeling components. Background in Python/Matlab/COMSOL will be beneficial.	

Only those candidates who have external fellowships like CSIR/DBT JRF can opt for the following topics [12(JB) to 24(SMe)]

12(JB)	Only FA	jb@iitb.ac.in	Jayesh Bellare	Bio-carbon development and assessment for molded automotive polymer components	To prepare bio-carbon from agro sources like coffee chaff, rice husk, coconut coir, and almond husk, and to blend it with Polypropylene, Polyethylene and Poly lactic Acid polymers for molded automotive polymer components	Includes both, experiments and modeling	Plastics technology specialization after first degree in chemical engineering or chemistry.	See for example: Polymers 2021, 13(16), 2663; https://doi.org/10.3390/polym13162663
13(AbM)	Only FA	abhijtm@iitb.ac.in	Abhijit Majumder and Jyoti Seth	Understanding the role of tissue viscoelasticity in breast cancer	<ol style="list-style-type: none"> 1. To prepare and characterize viscoelastic materials for cell culture. 2. To study the effect of substrate viscoelasticity on the proliferation, invasion, migration, and drug sensitivity of the breast cancer cells. 3. Pathway analysis to understand the molecular mechanism of viscoelasticity sensing. 4. To develop a theoretical model for cell migration in response to viscoelastic and elastic cues. 	Includes both, experiments and modeling	Either Chem Engg or Bio. Depending on the background, the student will be working more on experimental or modelling aspect.	https://www.sciencedirect.com/science/article/abs/pii/S1742706121005729 https://www.sciencedirect.com/science/article/abs/pii/S0006291X21000520 https://www.sciencedirect.com/science/article/abs/pii/S2589152920303847
14(GK)	Only FA	guruswamy@iitb.ac.in	Guruswamy Kumaraswamy	Direct Ink Writing 3D printing using Colloidal Inks	3D printing or additive manufacturing involves building complex structures through a layer-by-layer process of deposition. Current methods include extrusion based methods such as Fused Deposition Modeling (FDM), UV cure and laser sintering methods. Each of these is specialized for a specific material (such as FDM and UV cure for plastics, laser sintering for plastics and metals). In this project, we will develop DIW methods, which is an extrusion technology to print materials starting from a variety of colloidal inks.	Experimental	Chemical Engineering, Physics or Chemistry - preferably with some knowledge of soft materials, colloids	
15(SS)	Only FA	saini@che.iitb.ac.in	Supreet Saini	Experimental evolution of metabolic cooperation.	In a strictly Darwinian sense, only traits that enhance an individual's fitness are selected. However, we know from experience, that cooperation between individuals/populations/species is ubiquitous in nature. How then do we explain evolution of cooperation? In this project, we will design evolutionary experiments to study evolution of cooperation between populations and between species.	Experimental	Any background with a strong interest in evolutionary biology.	
16(SS)	Only FA	saini@che.iitb.ac.in	Supreet Saini	Investigation of factors dictating rate at which new species form.	Species diversity across the globe is quite non-uniform (https://en.wikipedia.org/wiki/Species_richness), with the tropics hosting considerably greater number of species per area. Using yeast and bacteria, we will design and perform evolutionary experiments to identify the key features which determine this spread of species diversity.	Experimental	Any background with a strong interest in evolutionary biology.	

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17(RB)	Only FA	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	Polymer particle size distribution and its dispersion stability during synthesis	<p>The objective of the research is to increase the stability and loading (in wt.%) of solid, polymer particles, in a solid-liquid (water) dispersion of these particles, during synthesis. This concentrated dispersion is expected to have a controlled, unimodal particle size distribution, to facilitate subsequent existing applications of the polymer.</p> <p>Polymer particle size (in tens of microns), particle volume fraction and viscosity of dispersion are parameters that might help to achieve stability at high polymer loading. In this research, one has to model and simulate, coupled computational fluid dynamics (CFD) of the reactor-mixer flow-field, with kinetic Monte Carlo or population balance equation (PBE) based models, to calculate size distribution of polymer particles. One can validate the simulation results with experimental data available in literature or our in-house data.</p>	Includes both, experiments and modeling	(i) MTech/ME/BTech/BE in Chemical/Mechanical/Polymer/Materials Engg. or allied Engg. branches or (ii) MSc in Physics/Chemistry/Materials Sc. or allied basic science depts.	
18(GAV)	Only FA	ganeshav@iitb.ac.in	Ganesh Viswanathan	Discrete kinetic modeling of TNFa signaling network	<p>Tumor Necrosis Factor alpha (TNFa), a pleiotropic cytokine involved in multiple phenotypes, is strongly implicated in many diseases such as cancer and autoimmune disorders such as arthritis. Dynamics of the biological network triggered by TNFa must contain signatures corresponding to the cellular response. The goal of this project is to use systems biology approaches to model this dynamic regulation. The project will involve construction of the underlying reaction network and develop discrete kinetic model to discern the regulatory effects.</p>	Theoretical/Computational	B.Tech/M.Tech Biotechnology or Chemical Engineering or equivalent; M.Sc Physics (with interest in Biology). Experience in Matlab or Python coding preferred.	https://www.che.iitb.ac.in/web/faculty/ganesh/pdfs/2021/booleanModelingCancerSignalingNetworks.pdf
19(RB)	Only FA	rajdip@che.iitb.ac.in	Rajdip Bandyopadhyaya	An Autonomous Water Quality Monitoring System for Water bodies	<p>We have been developing a complete water quality monitoring system consisting of a core module hosting an array of electrode/optical probe-based sensors for monitoring standard water-body parameters such as pH, temperature conductivity, turbidity, oxidation-reduction potential (ORP), dissolved oxygen (DO) etc., and reagent based quantification modules for specific chemical pollutants (e.g., fluoride - an inorganic pollutant, arsenic and chromium - metal pollutants etc.).</p> <p>Additional sensor modules can be installed to the core module, when required for a specific water body. The station is IOT enabled, and sensor readings are relayed to a wireless gateway at periodic intervals, which should be accessible anywhere in the world through a web interface. The entire system is envisaged to be locally powered at the deployment site, by a solar panel-battery combination, with uninterrupted operation over several weeks, without any manual intervention.</p> <p>One has to work in an interdisciplinary team and it will involve nanomaterials, 3D manufacturing and electronics as research areas.</p>	Experimental	(i) BTech/BE/MTech/ME in Chemical/Electrical/Mechanical/Materials Engg. or allied areas or, (ii) MSc in Physics/Electronics/Materials Sc. or allied areas	
20(SMe)	Only FA	sarika@che.iitb.ac.in	Sarika Mehra	Genome scale metabolic analysis of recombinant CHO cells for improved fitness and product titers	<p>A large number of therapeutics used to treat a wide range of diseases are recombinant proteins, that require mammalian cells as a host for their commercial production. Chinese hamster ovary (CHO) cell lines are the most preferred host cells for the production of a variety of biotherapeutics ranging from interferons to antibodies. The increasing demand to treat a variety of diseases has necessitated the need to increase the overall productivity of these therapeutic proteins. One of the bottlenecks in increasing productivity is the processing of proteins in the ER (endoplasmic reticulum) before secretion. Data from our lab has demonstrated the potential of an approach, based on adaptive laboratory evolution, to adapt cells to ER-stress and thus achieve high titers of a monoclonal antibody. In this project, we aim to understand the impact of this approach on the metabolic fitness of the adapted cells using a combination of experiments and modelling such as genome scale metabolic models.</p>	Includes both, experiments and modeling	Chemical Engg/Biotechnology, background in basic mathematics is desirable.	
21(SMe)	Only FA	sarika@che.iitb.ac.in	Sarika Mehra	Integrate protein-DNA interaction network with genomic data to predict the impact of mutations in clinical strains of M. tuberculosis.	<p>In spite of significant medical advances, tuberculosis (TB) is a major killer worldwide. In India alone, more than 12 lakh people are diagnosed with tuberculosis every year, with 2.7 lakh resulting in death. 40% of these cases are children. The major problem with conventional tuberculosis therapy has been the emergence of multi-drug resistance (MDR) and extensively drug resistance (XDR) Mycobacterium tuberculosis strains. Whole genome sequencing of many clinical strains show a number of mutations present in these clinical strains. In this project, we will represent the regulatory network of this bacteria in a Boolean framework. To determine the Boolean function at each node, gene expression data will be utilized along with in-house developed algorithms. The model will be simulated to predict the impact of various mutations that are seen in clinical strains of drug-resistant M. tuberculosis.</p>	Theoretical/Computational		
22(HN)	Only FA	hnanavati@iitb.ac.in	Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers (TA / FA)	<p>In this project, the aim is to understand quantitatively the molecular elasticity of biopolymers with potential engineering applications. The first example is Spider Dragline Silk, which may be several times stronger than steel (after normalizing the density). The work involves experimental, computational and theoretical analyses of the molecular structure of the biopolymer system.</p>	Includes both, experiments and modeling	Chemical Engg./Chemistry/Physics/Materials Science/Polymers/Knowledge in coding	
23(HN)	Only FA	hnanavati@iitb.ac.in	Hemant Nanavati	Accurate Molecular Models for Real Polymers (TA/FA)	<p>We develop compact, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects.</p> <p>The applications include synthetic as well as high performance Bio-sourced polymers.</p>	Theoretical/Computational	Chemical Engg./Chemistry/Physics/Materials Science/Polymers/Knowledge in coding	
24(SMe)	Only FA	sarika@che.iitb.ac.in	Sarika Mehra	Understanding the role of dehydrogenases in anti-microbial resistance	<p>Evolution of Mycobacterium smegmatis, a model organism for development of resistance in M. tuberculosis, led to the SNPs in various dehydrogenase genes. In this project, we aim to understand the role of these mutations using gene knockout, allele exchange and systems biology tools.</p>	Experimental	A knowledge of molecular biology techniques such as cloning would be preferable.	