

"Department of Chemical Engineering, IIT Bombay.  
Preference for TA, TAP and FA Ph.D Topics for Spring, 2022-2023  
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Project Code	Type of the project (TAP, TAP or FA, FA only)	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, etc.):	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(RaD)	Only TAP	dasgupta.ratul@iitb.ac.in	Ratul Dasgupta	Wind generation of ocean waves: from primary instabilities to cyclogenesis	<p>Wind blowing over the flat ocean surface destabilises it, producing waves which can range from ripples (wavelength of a few millimetres) to surface gravity modes, tens of metres long. The formation of these causes the sea surface to become rough and this roughness in turn significantly affects the momentum flux as well as sensible and latent heat flux, from the ocean to the atmosphere. In addition, the breaking of some of these waves can lead to a complex sequence of processes which eventually produce ejection of fluid particles from the ocean surface (sea spray) with sizes spanning submicrons to millimetres. When the wind speed exceeds about 32 m/s, the heat flux from the ocean surface and the accompanying spray, is thought to play a crucial role in suppressing the turbulent intensity or intensifying air circulation above the ocean surface, potentially giving birth to cyclones.</p> <p>The aim of this project is to conduct extensive Direct Numerical &amp; Large Eddy Simulations for studying the effect of breaking waves due to wind on the ocean surface leading to spray formation and the thermodynamics of the spray generated. This is a joint project between IIT Bombay, IIT Ropar and IIT Madras) funded by SERB-DST involving rigorous theoretical, computational and experimental work. An experimental facility for wave breaking is under development at IIT Ropar (Prof. Devranjan Samanta, Mechanical Engg.). The project will be collaborative in nature working closely with the groups of Prof. Anubhab Roy (IIT Madras, Applied Mechanics) and Prof. Devranjan Samanta at IIT Ropar. Please apply if you think you are strong in physics and maths and wish to learn theoretical techniques in fluid mechanics, CFD using open source codes as well as programming.</p>	Theoretical/Computational	Mechanical/Aerospace/Chemical Engg., MSc Physics with strong background in theory, Exposure to programming and CFD is highly desirable	
3(JA)	Only TAP	adhikari@iitb.ac.in	Jhumpa Adhikari	Molecular Simulation and Experimental Studies on Thermodynamics of High-Value Biochemicals derived from Biomass Valorization	The project is through CoE:OGE, IIT Bombay with IOCL as industry partner and involves use of molecular simulations (at IIT Bombay) and experiments (at IOCL) to study the thermodynamics of high-value biochemicals derived from biomass valorization.	Includes both, experiments and modeling	Chemical Engineering, Knowledge in coding	
4(YS)	Only TAP	yshastr@iitb.ac.in	Yogendra Shastr	Decision support system for optimal regional mapping of agricultural residue and end uses	Multiple applications of agricultural residue such as bio-power, ethanol, and biogas production are proposed in India. The economic and environmental feasibility of these options is regional. It depends on local residue availability, scale, seasonality, regional energy requirements and so on. In this project, we will develop a strategy to identify optimal regional mapping between residue and end uses. Detailed economic assessment of selected technologies will be done. Environmental impacts such as water footprint, carbon footprint, and air pollution will be calculated. This information will be used to recommend region specific (district or state level) utilization options for residue. An interactive decision support system that makes this platform accessible to interested users may also be developed.	Theoretical/Computational	Chemical engineering, Biotechnology, Industrial engineering, operations research, mechanical engineering. The work will require computer programming. Experience in computer programming is desirable but not a requirement.	<p>Prior work in this area considering only ethanol as product and using only cost as the criteria for Maharashtra can be found at: <a href="https://link.springer.com/article/10.1007/s10098-021-02227-4">https://link.springer.com/article/10.1007/s10098-021-02227-4</a></p> <p>The proposed project will extend this work to include additional uses, more regions in India, and other factors such as water footprint and pollution generation.</p>
5(JS)	TAP or FA	lyotseth@iitb.ac.in	Jyoti R. Seth	Gel Based Propellants	<p>Gel based propellants contain suspended oxidisable nanoparticles in the fuel matrix that enhance the energy density of these fuels. Such propellant systems behave as viscoelastic gels during storage and their viscosity decreases under shear during the feeding process. Atomisation then forms propellant droplets containing energetic nanoparticles. Ultimately, high calorific value of the nanoparticles (such as boron) offers increased flight performance of the propulsion vehicles.</p> <p>The current project studies various aspects of gelled fuels with suspended oxidisable nanoparticles from manufacture to use. The project will involve implementing a process to develop a stable and energy dense gelled fuels for use in a combustion set-up. Performance of these gelled fuels will be studied through its flow and rheological properties, atomisation and combustion behaviour. Lab-scale experiments will be followed by scale-up and technology transfer of the production process.</p>	Includes both, experiments and modeling	Chemical Engineering, Chemistry, Mechanical Engineering, Physics	

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6(OM)	Only TAP	ojus@iitb.ac.in	Ojus Mohan	Catalytic hydrogenation of carbon dioxide to higher hydrocarbons	CO2 conversion into value-added products has the advantage of lowering CO2 emissions and producing beneficial chemicals. The conversion of CO2 to C1 molecules including methane, methanol, formaldehyde, etc. has been the subject of extensive investigation in recent years. Comparatively, there aren't many studies on producing C2 hydrocarbons (ethanol, DME, etc.) from CO2 hydrogenation. The main impediment is finding a catalyst with exclusive selectivity to C2 products at high CO2 conversion rates. The catalyst needs to have a few desirable qualities, like a low CO2 activation barrier, low selectivity toward methane (suppress complete hydrogenation), and the ability to promote C-C coupling. The problem of successfully creating an active and selective catalyst for the CO2 hydrogenation to C2 products remains unsolved and is the current bottleneck in commercializing this process. The proposed combined computational and experimental study aims to establish a clear correlation between the intrinsic properties of catalysts and their CO2-activation and C-C coupling ability to design novel catalysts for this process. The strategy is to computationally screen the existing popular catalysts for this reaction (employing state-of-the-art quantum computational tools) based on the above characteristics and provide mechanistic insights into the CO2 conversion reaction. The knowledge gained from these computational studies will guide in synthesizing more efficient catalysts for this reaction and eventually bring this technology from research laboratories to industry.	Includes both, experiments and modeling		
7(YS)	Only TAP	yshastri@iitb.ac.in	Yogendra Shastri	Studies on the effect of pre-treatment options on CBG production from Biomass	Pretreatment of agricultural residue is very important to improve yield of biomass in anaerobic digestion so that production of compressed biogas (CBG) becomes economically feasible. In this work, we will study different pre-treatment options and their effects on the biogas yield. Starting with information about different technologies available in literature, the may also involve conducting experiments for selected options with industry collaborators. Based on the data collected/generated, economic and life cycle analysis will be done and optimal pre-treatment option will be recommended. This project is in collaboration with industry partner (Indian Oil Corporation Limited).	Includes both, experiments and modeling	Chemical Engineering, Biotechnology, Chemistry. Prior experience in process design and optimization is desirable but not essential.	
8(RT)	Only TAP	rochish@che.iitb.ac.in	Rochish M Thakkar	" Studies on particle scavenging characteristics by ElectroHydroDynamic (EHD) Sprays and the development of a filterless Aircleaner System"	The use of charged droplets to treat pollutants and combustion products has been described in the literature since 1940s. It overcomes the problem of high pressure-drop in filtration and ozone generation in electric based air purification systems. The project aims at both, developing a fundamental understanding of interaction between charged droplets and aerosol particles and based on this learning building a prototype electro-spray based air cleaner. The project would essentially involve conducting a series of experiments on understanding fundamentals of droplet-particle interaction, using an in-house levitation device, namely the electrodynamic quadrupolar trap. Charged droplets and aerosols interact via hydrodynamic as well as electrostatic interaction. These understandings will be used to develop a scaled up electro-spray air cleaner. The essentials will involve developing a well formed electro-spray, particle injection system, using instruments to quantify particle capture amongst others.	Includes both, experiments and modeling	Chemical, Mechanical Engg, No prior knowledge required	<a href="https://www.che.iitb.ac.in/faculty/rochish-madhukar-thakkar">https://www.che.iitb.ac.in/faculty/rochish-madhukar-thakkar</a>
9(RT)	Only TAP	rochish@che.iitb.ac.in	Rochish M Thakkar	Theoretical investigations on the fundamentals of particle-droplet interactions and the development of a mathematical model for optimizing the performance of an ElectroHydroDynamic (EHD) Spray based air cleaner system.	The development of an air cleaner system using ElectroHydroDynamic (EHD) Sprays is being undertaken in our laboratory. The PhD work associated with this development will involve conducting boundary element and other CFD studies to obtain a fundamental understanding of the charged droplet-particle interaction processes. Towards this end, existing inhouse codes, new inhouse codes, and commercial CFD softwares will be used. Further, this understanding will be applied towards the development of a mathematical model to arrive at an optimum design for the prototype electro-spray based air cleaner system. The models will involve particle capture efficiencies, hydrodynamics and electrostatics, population balance modeling and CFD studies.	Theoretical/Computational	Chemical, Mechanical, Physics	<a href="https://www.che.iitb.ac.in/faculty/rochish-madhukar-thakkar">https://www.che.iitb.ac.in/faculty/rochish-madhukar-thakkar</a>
22(AbM)	TAP or FA	abhijtm@iitb.ac.in	Abhijit Majumder and Debjani Paul (BSBE)	Tumor on Chip	Understanding tumor growth on dish has always been a challenge for its complex nature. It involves cell to cell contact between multiple cell types, complex tissue 3D architecture, tissue rigidity, designing nearby blood vessels etc. In the proposed work, we plan to develop "Tumor on Chip." The project will have multiple parts such as developing blood vessels on chip, developing tumor micro-environment, and then finally assembling all the parts together. The model developed will help us in testing drugs for their ability to cross blood-brain barrier ( <a href="https://en.wikipedia.org/wiki/Blood%E2%80%93brain_barrier">https://en.wikipedia.org/wiki/Blood%E2%80%93brain_barrier</a> ).  The work will involve microfluidics, micro-fabrication, and cell culture.	Experimental	Bio with interest in engineering	

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23(MT)	Only TAP	mahesh@che.iitb.ac.in	Mahesh Tirumkudulu	Controlled Drug Delivery in Oral Osmotic Tablets: Modelling	The project deals with the mathematical modeling of the drug release process in oral osmotic tablets, which ensures a controlled delivery of the drug inside the body. We have established a tablet manufacturing facility in our lab where we manufacture oral osmotic tablets. As part of the project, We are also studying the in-vitro dissolution process of the tablets. The prospective student would study the flow and mass transfer processes to arrive at a detailed mathematical model of the entire process. We have an ongoing collaboration with Pfizer Inc. and the student would be part of the IITB-Pfizer team studying this problem.	Theoretical/Computational	Strongly fundamentals in Chem Engg.	The link to a recent work from our group is here: <a href="https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4177752">https://papers.ssrn.com/sol3/papers.cfm?abstract_id=4177752</a>
24(SBH)	Only TAP	sharad_bhartiya@iitb.ac.in	Sharad Bhartiya	Quasi-linear Parameter Varying Systems Representation and Control of Nonlinear Chemical Processes: A Machine Learning Approach	The most sophisticated control systems that exist today combine adaptive or learning components with predictions of the future behavior in their decision making processes. The way forward is to obtain a mathematical representation of the underlying process, often called, the digital twin and interrogate this to obtain path forward. There are three obstacles in such an approach: (1) accurate digital twins are difficult to obtain for most problems of interest and require huge investment of resources and time, and (2) even if one becomes available, the calculation of the optimal control problem in presence of constraints for a complex math representation is impractical for time-critical real time applications, (3) the digital twin itself becomes outdated and therefore routinely needs to be updated to have a sustainable impact. This work attempts to address the first and last of these obstacles using machine learning approaches and the second obstacle is addressed using simpler linear like constructs for the digital twin.	Theoretical/Computational	Chemical / Electrical / Instrumentation and control, dynamic systems/ Machine Learning	
25(SME)	TAP or FA	sarika@che.iitb.ac.in	Sarika Mehra	Engineering rCHO cells to increase titers of monoclonal antibodies and vaccine protein sub-units	A large number of therapeutics used to treat a 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. Similarly, many vaccine candidates, such as the receptor binding domain of the SARS-COV2 are also produced in mammalian cells due to their glycosylation. The pandemic highlighted the need to shorten the clone development timelines for rapid production of antibodies and vaccine candidates. Productivity of such secretory proteins is a multifaceted phenomenon, requiring integration at a transcriptionally active site, a well-coordinated signaling network between different metabolic pathways, including protein secretion, to secrete functionally active proteins out of the cells. In this project, we aim to develop a systems level understanding of pathways that contribute to high productivity of cell lines to generate a host CHO cell line that is engineered for increased secretion.	Experimental		
26(AbM)	TAP	abhijtm@iitb.ac.in	Abhijit Majumder	To Study the Role of Substrate Viscoelasticity in the Migration of Breast Cancer Cells".	1. To prepare and characterise materials with different viscoelasticity. 2. To understand the effect of viscoelasticity of the tumor microenvironment on breast cancer cells and their migration. 3. To model the observation obtained in objective 2.	Includes both, experiments and modeling	Chemical Engg or Biotech	
<b>Only those candidates who have external fellowsip/s like CSIR/DBT JRF can opt for the following topics [10(HN) to 21(SMe)]</b>								
10(HN)	Only FA	hnanavati@che.iitb.ac.in	Hemant Navavati	Accurate Molecular Models for Real Polymers (TA/FA)	We develop compact, closed form, but accurate molecular models as well as elasticity relationships for real polymers, incorporating structural aspects.  The applications include synthetic (e.g., those used as matrix for solid propellant) as well as high performance Bio-sourced polymers.	Theoretical/Computational	Chemical Engg/Chemistry/Physics/Materials Science/Polymers/Knowledge in coding	
11(HN)	Only FA	hnanavati@che.iitb.ac.in	Hemant Navavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers (TA / FA)	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.	Includes both, experiments and modeling	Chemical Engg/Chemistry/Physics/Materials Science/Polymers/Knowledge in coding	

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12(JS)	Only FA	joytiset@iitb.ac.in	Jyoti R. Seth	Three-dimensional Self Assembly of Graphene	<p>Three-dimensional (3D) graphene is known to have numerous applications as adsorbent, catalysts, sensors, energy storage such as batteries and super-capacitors. Further, 3D graphene is easy to handle and convenient to load as adsorbent in a packed bed. One of the ways of preparing 3D graphene is through reduction of 2D graphene oxide particles which leads to self-assembly of the reduced graphene particles in to a 3D "house of cards" type structure. However, this resultant structure has to have mechanical strength as well as flexibility and compressibility so that it is amenable to be used as packing in large scale industrial columns. At the same time, the surface area of the original 2D graphene oxide must be preserved, to the extent possible, so that the properties of 2D graphene such as conductivity and surface area are conserved.</p> <p>The aim of this PhD topic would be to develop techniques for preparation of 3D graphene in order to achieve desired characteristics as mentioned above. Influence of methods of reduction, types of reducing agents, kinetics of reduction and various other parameters on the number as well as strength of connections between reduced graphene particles will be studied. The dynamics of the self-assembly will also be studied through an analogous experimental system involving 3D printed sheet-like particles representing graphene. Embedded magnets in the particles will be used to tune particle-particle attraction. This work is in collaboration with Dr. Per Loethman of Foviatech GmbH (<a href="https://www.foviotech.com">https://www.foviotech.com</a>). The selected student may spend some time at our collaborator's lab in Germany. A collaboration with University of Delft in Netherlands is also foreseen.</p>	Includes both, experiments and modeling	Physics, Chemistry, Material Science, Mechanical or Chemical Engineering	<a href="https://www.che.iitb.ac.in/phd-ta-topic/three-dimensional-self-assembly-graphene">https://www.che.iitb.ac.in/phd-ta-topic/three-dimensional-self-assembly-graphene</a>
13(RB)	Only FA	rajdip@che.iitb.ac.in	Rajdip Banyopadhyaya	Development of polymeric implant for nanoparticle mediated drug delivery in pancreatic cancer	<p>Pancreatic cancer is one of the cancers having the lowest 5-year survival rate, because of its late diagnosis and availability of only a couple of known drugs with very moderate increase in patient's survival. Based on our earlier work, we have shown that, nanoparticle mediated delivery of existing drugs can enhance the cytotoxicity in cancer cells. Accordingly, we have developed subcutaneous and orthotopic in-vivo experiments in mouse, in collaboration with Advanced Cancer Teaching Research and Education Centre (ACTREC), Navi Mumbai.</p> <p>The aim of this project will be to further increase the efficacy of this process, by making 3D printed, polymer-based implants in order to mimic the interaction of nanoparticles with cancer cells in a controlled microfluidic environment. The resulting insight will elucidate the optimization of the nanoparticle-based drug delivery system.</p> <p>Some background or experimental exposure in any of the following is better: polymeric materials or nanomaterials or microfluidics or drug delivery, Chemical Engineering principles like transport phenomena, reaction engineering and life-sciences oriented skills in cell cultures, drug loading, release, cell dynamics will be useful.</p> <p>The project is funded by WRCB, IIT Bombay and it will be a work leading to learning and expertise in interdisciplinary research areas in chemical engineering, material science and biotechnology. The work will be in a group of students involving others already working in related parts of this project.</p>	Experimental	Chemical Engg., Materials Sc. & Engg., Biosciences & Bioegg.,	
14(SBN)	Only FA	noronha@iitb.ac.in	Santosh Noronha	Enzyme bioreactors	The objective is to design and implement catalytic bioreactors. Work elements will involve standardization of a catalytic system, characterization of kinetic and transport aspects, process optimization, and detection in real time.	Includes both, experiments and modeling	Exposure to process reaction engineering and/or biocatalysis would be an advantage.	
15(GAV)	Only FA	ganeshav@iitb.ac.in	Ganesh Viswanathan	Modeling cell death	Cell-death process, which occurs ubiquitously under normal and healthy conditions, is disturbed in diseased tissues. Cell-death process can be viewed as an outcome of a network of biochemical reactions. How does the network dynamically orchestrate the overall cell-death outcome? Can the network be re-wired to reverse the disturbances in the cell-death process? The goal of this project is to understand the cell-death process by developing a kinetic model of the underlying network and validating with the experimental measurements. The project will involve simulating the model to generate big data and analysing the same using appropriate tools.	Theoretical/Computational	Chemical Engg./Mechanical Engg./Physics/Biotechnology/Biochemical Engg./Systems biology. No prior background in biology needed. Interest to learn and collaborate with experimentalists is desired.	Matlab and/or Python toolboxes will be used for simulations. Experimental data is available in-house. Recent manuscript: <a href="https://www.che.iitb.ac.in/web/faculty/ganesh/pdfs/2022/modulation.pdf">https://www.che.iitb.ac.in/web/faculty/ganesh/pdfs/2022/modulation.pdf</a>
16(GAV)	Only FA	ganeshav@iitb.ac.in	Ganesh Viswanathan	Modeling phenotype switching	Tumor necrosis factor alpha (TNFa), a pleiotropic cytokine is implicated in several pathological conditions. TNFa is an important component of the cytokine storm observed in COVID19 patients causing strong lung-inflammation. TNFa is capable of making the triggered cells take different phenotypes such as pro-survival or apoptotic or necroptotic state. Why and how cells permit multiple phenotypic responses? Can the underlying signal transduction network consisting of biochemical reactions be modulated dynamically to enable phenotype switching? The objective of the project is to develop systems biology based models of the network to identify strategies for phenotype switching from pro-survival to apoptosis/necroptosis. The project will primarily involve modeling and simulations, and subsequently contrasting the model predictions with experimental data.	Theoretical/Computational	Chemical Engg./Mechanical Engg./Biotechnology/Physics. No prior background in biology needed. Interest to learn and collaborate with experimentalists is desired. Knowledge in coding in Matlab/Python.	<a href="https://www.che.iitb.ac.in/web/faculty/ganesh/pdfs/prePrint/boolean.pdf">https://www.che.iitb.ac.in/web/faculty/ganesh/pdfs/prePrint/boolean.pdf</a>

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17(SS)	Only FA	saini@che.iitb.ac.in	Supreet Saini	Evolutionary dynamics of antibiotic resistance in bacteria.	Resistance to antibiotics arises in the span of a few generations in bacterial populations. Despite several experiments having demonstrated this, we have little conceptual understanding of the dynamics of the process of evolution of resistance. In this project, we will develop a conceptual framework in which to understand evolution of resistance. In particular, we will aim to predict if/when a particular strain can acquire resistance to a particular class of antibiotics.	Theoretical/Computational	Any background with a strong interest in evolutionary biology.	
18(SS)	Only FA	saini@che.iitb.ac.in	Supreet Saini	How does innovation arise in biological design?	Many facets of organismal physiology (like flight, eyes, development) have evolved seemingly from scratch, with seemingly no evolutionary intermediates. However, to what extent does evolution proceed by refurbishing and reshuffling existing genes; and to what extent by evolution of new genes? In this project, we will study pathways and genes across species from a broad range of phyla to help answer this question.	Theoretical/Computational	Any background with a strong interest in evolutionary biology	
19(SMe)	Only FA	sarika@che.iitb.ac.in	Sarika Mehra	Development of engineered cell lines for rapid production of recombinant proteins and vaccines	The current pandemic highlighted the need to rapidly develop stable cell lines for the production of monoclonal antibodies and other therapeutics for clinic testing and beyond. Biotherapeutics and biosimilars are produced in mammalian hosts, primarily CHO cells, due to their complex glycosylation that is critical for their function. In recent years, HEK293 cell line is being explored and developed for production of many proteins where human like glycosylation is essential. In this project, we will use cell engineering approaches to develop improved host cell lines for high and rapid production of recombinant proteins.	Experimental		
20(AbM)	Only FA	abhijtm@iitb.ac.in	Abhijit Majumder and Jyoti Seth	Understanding the role of Substrate Rheology on breast cancer metastasis	In this work, we wish to explore the role of rigidity and loss modulus on the migration of breast cancer cells. For this purpose, migration of invasive and non-invasive breast cancer cells will be studied on the gels of different combinations of G' and G". An attempt will be made to understand the migration mechanism in response to substrate viscoelasticity and deformation. This proposed work will provide us fundamental understanding about migration in breast cancer and will help in finding new therapeutic targets. Additionally, the insight gained should be applicable for other pathophysiological conditions that involve cellular migration.	Includes both, experiments and modeling	Chemical Engg interested in Biology/Bio background	1. "Viscotaxis"-directed migration of mesenchymal stem cells in response to loss modulus gradient" 2021 Acta Biomaterialia 2. Viscoelastic substrate decouples cellular traction force from other related phenotypes, 2021, BBRC 3. Substrate loss modulus promotes the differentiation of SHSY-5Y neuroblastoma cells 2020 Materialia.
21(SMe)	Only FA	sarika@che.iitb.ac.in	Sarika Mehra	Design of treatment protocols to counter emergence of resistance	Our group has been working on various aspects of antibiotic resistance, specifically in the context of tuberculosis. We use adaptive laboratory evolution with whole genome sequencing to identify mechanisms of resistance. The experiments are combined with mathematical models to predict evolution of resistance. In this project we will design and test how drug dosage parameters influence the emergence of resistance.	Includes both, experiments and modeling		