TAP topics

Name of Faculty	Title of PhD topic	Project code	Area of the research (One key word)	Nature of the project (Experimental/Modeling/Theoretical/):	Objectives (4-5 lines): You may provide a link to the additional information (Additional description, videos etc.) [Optional]	Background required (e.g. Chemical Engg/Chemistry/Physics, Specific experimental expertise/Knowledge in coding, etc.):
Sayantan Dutta	Computational Model of self-assembly and dynamics of biomaterials	SyD-TAP	Biophysics/Soft Matter	Theoretical / Computational / Modelling	Our group works on building computational models for self-organization in biological systems across scales with a vision of writing down the design principles of functional biomaterials. We use multiple tools of engineering and applied physics as the problem in hand needs. The specific problem will be decided based on the mutual interest of the student and the PI. Some example problems currently our group is interested are: (i) Developing a particle-based simulation framework to study three dimensional self-assembly of cells. (ii) Developing a framework for designing artificial tissue driven by mechanical and chemical patterns. (iii) Developing a model for self-assembly of cells by long-range interaction of cells. (iv) Adapting the physics of flexible polymers to understand chromatin dynamics.	Ideal background--Physics/Core Engineering. A passion for problem solving and strong quantitative/computational skill is required. No Biology background is required.
Guruswamy Kumaraswamy	Molecular Mechanisms of Micro-Nanoplastic Formation	GK-TAP	Microplastics	Experimental	Secondary microplastics are small plastic fragments (< 5 mm in size) that form due to weathering of large plastic objects during use. These have now been recognized as a particulate pollutant and are observed to be ubiquitous. This has consequences for the environment and for human health. This project (funded by ANRF) is focused on understanding the molecular mechanisms of microplastic formation. Our previous work has focused on microplastic formation due to environmental weathering (for example, due to exposure of plastics to UV and sunlight: see: Nat. Commun. 2025, 16, 3051) and due to mechanical stress (Soft Matter. 2025, 21, 2782-2786). This project will employ a range of experimental tools (light scattering, X-ray diffraction, rheology) and will use model systems (synthesized by our collaborators in NCL) to understand fundamental principles of microplastic formation.	Chemical Engineering; Materials Science; Some exposure to soft materials and experimental materials characterization (Scattering, rheology, DSC) is desirable
Ateeque Malani	Decarbonization using Red-Mud Soil : Combined Modelling and Experimental Study (Co-guide, Prof. D N Singh from Civil Dept)	AtM-TAP	Decarbonization, gas adsorption, storage	Both: Theoretical (Computational or Modelling) + Experimental	This study investigates the potential of red mud, an industrial byproduct of alumina production, as a low-cost and sustainable material for carbon dioxide (CO_2) capture and decarbonization. Earlier studies have shown that red-mud has great potential for CO2 storage, however many aspects of this carbon capture and storage has not been explored. In this project, the goal is to probe the CO2 adsorption capacity of red-mud, and effect of various parameters such as pH, moisture content and red-mud composition on long-term storage capacity.	Strong motivation and perseverance is more important. Enthusiastic student with background in Chemical Engineering, Physical Chemistry, Mechanical Engineering, Materials Engineering can apply.
Sonali Das	Catalyst and process development for low-temperature onboard NH3 decomposition coupled with NH3-H2 engines	SD-TAP	Catalysis & Reaction Engineering	Both: Theoretical (Computational or Modelling) + Experimental	Green hydrogen is crucial for a sustainable energy future, but storing and transporting it safely is a major challenge. This project explores an alternative approach—using ammonia as a hydrogen carrier and releasing hydrogen when and where it is needed. You will work on catalyst development and reaction engineering for low-temperature ammonia decomposition, including both thermo-catalytic and light-assisted routes. The project also involves process modeling and integration with NH_3–H_2 engines to evaluate real-world performance. https://sites.google.com/view/das-lab	Chemical Engineering

TAP topics

Jyoti Seth	Microstructure and Rheology of Particle Networks at Fluid-Fluid Interfaces	JS-TAP		Both: Theoretical (Computational or Modelling) + Experimental	While the interfacial rheology of particle-stabilized emulsions and foams is well-established, most studies are fragmented, focusing either on introduced colloidal particles (e.g., silica, polystyrene) or in situ crystallizing species (e.g., monoglycerides, proteins). Further, real-time visualization of structural evolution under deformation remains technically challenging and underexplored. We seek to address this gap using a combination of experiments and simulations. In-house experimental setups will be designed and developed to enable simultaneous imaging of interfaces while probing their rheology.	Chemical Engg / Mech Engg / Material Science / Chemistry / Physics
Ganesh Viswanathan	Modeling TNFα mediated Cell death in chemoresistant Acute Myeloid Leukemia	GAV-TAP	Cancer systems biology	Both: Theoretical (Computational or Modelling) + Experimental	Acute Myeloid Leukemia (AML) is an aggressive and heterogeneous blood cancer, affecting predominantly older adults and children. Despite advances in understanding its molecular drivers and the development of targeted therapies, overall survival rate (typically < 50%) remains low. This could be attributed to acquired chemoresistance by AML tissue. Tumor Necrosis Factor α (TNFα), a pleiotropic cytokine abundantly present in the tumor microenvironment, is essential in driving uncontrolled tumor growth. The objective of this project is to develop experimental data constrained biochemical mathematical models of the TNFα mediated AML cell-fate response under chemoresistant conditions. Systematic model simulations contrasted with single-cell level experimental observations will be used to unravel the pathway mechanisms governing the cellular decision making and also to identify the targets to cell-fate modulation. In-house developed chemoresistant AML model cell lines and associated preliminary experimental data are already available. The project may involve both experimental and computational work. Basic programming skills desired.	Chemical Engineering/Biotechnology (or equivalent) with interest in cancer systems biology and basic knowledge of coding.
Mani Bhushan, Sujit Jogwar	Foundational Model to Aide Process Design Activity	MB-TAP	Process Systems Engineering	Theoretical / Computational / Modelling	Going from a production route concept, such as that embodied in a process flow diagram, to a detailed piping and instrumentation diagram is a challenging and iterative process. Currently it relies heavily on human expert involvement. This project will investigate AI driven approaches to automate significant proportion of this journey enabling the human expert to focus on key decisions. This will involve tools around digitization, multimodal language models, and incorporation of safety analysis methodologies such as Hazop during the design process. This project is in collaboration with a leading industrial partner.	Chemical Engg with interest in control, AI, and coding
Ratul Dasgupta	Direct Numerical Simulation of Turbulent Flows of Charged Suspensions	RD-TAP1	Fluid Mechanics	Theoretical / Computational / Modelling	The successful applicant will work with Prof. Ratul Dasgupta (co-PI) and Prof. Ravichandran's (PI) group at IIT Bombay to develop a numerical solver to study the dynamics of charged suspensions. Prior experience with direct numerical simulations (DNS) of the Navier-Stokes equations is required. Experience with code-development will be highly preferred.	Background: Physics or engineering, with interests in fluid dynamics and electrostatics.
Ratul Dasgupta	Fluid dynamics of droplet coalescence in clouds	RD-TAP2	Fluid Mechanics	Both: Theoretical (Computational or Modelling) + Experimental	This is a joint work with Prof. Anubhab Roy (IIT Madras, Applied Mechancs). The work will involve carrying out simulations and theory related to droplet coalescence in clouds.	Engineering (Chemical/Mechanical, Aerospace) or MSc Physics background

TA or FA topics

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Sayantan Dutta	Computational Model of self-assembly and dynamics of biomaterials	SyD-TA or SyD-FA	Soft Matter, Biophysics	Theoretical / Computational / Modelling	Our group works on building computational models for self-organization in biological systems across scales with a vision of writing down the design principles of functional biomaterials. We use multiple tools of engineering and applied physics as the problem in hand needs. The specific problem will be decided based on the mutual interest of the student and the PI. Some example problems currently our group is interested are: (i) Developing a particle-based simulation framework to study three dimensional self-assembly of cells. (ii) Developing a framework for designing artificial tissue driven by mechanical and chemical patterns. (iii) Developing a model for self-assembly of cells by long-range interaction of cells. (iv) Adapting the physics of flexible polymers to understand chromatin dynamics.	Ideal background--Physics/Core Engineering. A passion for problem solving and strong quantitative/computational skill is required. No Biology background is required.
Sudarshan Vijay	Accelerating materials discovery using noise-tolerant optimisation methods for quantum chemistry	SV-TA or SV-FA	Machine learning	Theoretical / Computational / Modelling	1. Find novel electro-catalysts and battery materials faster by improving the efficiency of first-principles methods 2. Develop and adapt noise-tolerant optimisation algorithms to rapidly locate minimum-energy structures, overcoming the instability caused by imprecise force evaluations 3. Construct a database of challenging chemical systems, such as charged surfaces and magnetic materials, to analyse and mitigate computational noise without increasing overall costs 4. Enable high-throughput materials discovery and machine learning integration by making calculations more robust, even when using modern, lower-precision hardware	Degrees in either Chemical Engineering, Chemistry or Physics. An interest in developing algorithms and production software.
Nagappan Ramaswamy	Energy Storage in Redox Flow Batteries	NR-TA or NR-FA	Batteries	Experimental	This project involves the study of vanadium redox flow batteries for long duration energy storage of renewable power sources such as solar and wind and development of new redox chemistries that enable higher energy densities.	Chemical engineering, Chemistry, Physics. Electrochemistry experience is preferred.
Nagappan Ramaswamy	Water Electrolyzers for Hydrogen Production	NR-TA or NR-FA	Electrochemical energy conversion and storage	Experimental	Development of materials and cell designs for electrolyzers such as Proton Exchange Membrane and Anion Exchange Membrane Water Electrolyzers. Work on aspects such as the performance, durability, hydrogen crossover of electrolyzers to decrease the eletrical energy consumption and levelized cost of hydrogen.	Chemical Engg/Chemistry/Physics. Electrochemistry experience preferred.
Ateeque Malani	Simulation Study of Enhanced Oil Recovery	AtM-TA or AtM-FA	Energy, Simulations	Theoretical / Computational / Modelling	Energy demand is increasing worldwide because of which extraction of crude-oil from existing matured oil-field is becoming more important. In mature oil fields, the crude-oil is strongly adhered to the rock surface. To remove this oil, additional chemicals needs to be supplied. In this project, we would use molecular simulations approach to probe the detachment of crude oil from rock surfaces using injecting fluids. This computational insight allows for the design of more efficient displacement fluids, bridging the gap between theoretical chemistry and field-scale production.	Hardworking, curiosity and interest in learning new things. Mathematical and coding skills are desirable.

TA or FA topics

Ateeque Malani	Modelling of early stages of cloud formation	AtM-TA or AtM-FA	Climate Change, Simulations	Theoretical / Computational / Modelling	The climate change is a reality which is creating extreme weather patterns of heavy rains and droughts which leads to loss of lives. The immediate reason is formation or absence of clouds in these events and hence understanding their formation is necessary. In this project, the focus is to probe early stages of formation of clouds in atmosphere by water condensation. Effects of various parameters would be explored.	Hardworking, curiosity, interest in learning new things. Mathematical and coding skills are desirable.
Ateeque Malani	Design of Porous Materials for Gas Storage and Separation	AtM-TA or AtM-FA	Gas Storage, Energy, Simulations	Theoretical / Computational / Modelling	Hydrogen and methane storage is a critical challenge for realizing their potential as a clean energy carrier, especially in mobile and portable applications. Carbon-based porous materials such as activated carbons, graphene derivatives, and metal-organic frameworks (MOFs) have shown promise in their storage due to their high surface area, lightweight nature, and chemical stability. By utilizing molecular simulations along with organic synthesis, our group seek to optimize the structural and functional properties of these materials to enhance their gas adsorption capabilities for both storage and separation purpose.	Hardworking, curiosity, interest in learning new things. Mathematical and coding skills are desirable.
Ateeque Malani	Design and Analysis of Clay-swelling Inhibitors	AtM-TA or AtM-FA	Energy, Simulations, Materials	Theoretical / Computational / Modelling	The petroleum industry is significantly challenged by clay swelling in subterranean formations, which occurs when hydrophilic clays absorb water, expanding in size and reducing the permeability of oil- bearing reservoirs. This phenomenon results in decreased oil recovery efficiency, increased production costs, and the potential for severe operational disruptions. Inhibiting clay swelling is therefore critical to improving oil extraction, particularly in shale and other clay-rich formations. Our aim is to use molecular simulations to rationally design inhibitors by analyzing structure-property relationships.	Hardworking, curiosity, interest in learning new things. Mathematical and coding skills are desirable.
Sonali Das	Catalyst and reactor development for sustainable light-assisted CO2 Utilization	SD-TA or SD-FA	Catalysis & Reaction Engineering	Experimental	This project focuses on converting CO_2 into valuable fuels and chemicals using dry reforming of methane. You will work on developing coke-resistant catalysts and explore photothermal approaches to drive the reaction more efficiently. The work will involve catalyst synthesis, advanced characterization, flow reactor experiments, and reactor design/ optimization. https://sites.google.com/view/das-lab	Chemical Engg./ Chemistry
Sonali Das	Catalyst and process development for Plasma-catalytic conversion of Methane to C2 hydrocarbons.	SD-TA or SD-FA	Catalysis & Reaction Engineering	Both: Theoretical (Computational or Modelling) + Experimental	Methane, a potent greenhouse gas, is often wasted through flaring. This project explores how it can be directly converted into more valuable fuels and chemicals using renewable electricity. You will work with non-thermal plasma and catalysis to enable methane conversion at low temperatures, addressing key challenges like energy efficiency and product selectivity. The project combines catalyst development, reactor design, and process modeling. https://sites.google.com/view/das-lab	

Sonali Das	Catalyst and Reactor development for Hydrogen production from Methane Pyrolysis	SD-TA or SD-FA	Catalysis & Reaction Engineering	Experimental	This project explores methane pyrolysis as a route to produce clean hydrogen, with solid carbon as a valuable co-product. You will work on developing advanced catalysts with high activity and resistance to deactivation, along with designing and operating reactors for high-temperature conversion. The project combines catalyst development, reaction kinetics, and reactor engineering, including studies on carbon formation and process optimization. It offers opportunities to work on both experiments and scale-up strategies for continuous, low-carbon hydrogen production. https://sites.google.com/view/das-lab	Chemical Engineering
Swati Bhattacharya	Using computer simulations to understand how diabetes develops and develop new therapeutics	SwB-TA or SwB-FA	Molecular Simulations	Theoretical / Computational / Modelling	As of 2026, approximately 9.6% of India's population aged 20 to 79 years is affected by diabetes, according to World Bank data. In absolute numbers, this translates to over 212 million people, making India the country with the highest number of individuals living with diabetes globally. The prevalence is higher in urban areas (11.2%) compared to rural areas (5.2%), and a significant portion of cases remain undiagnosed. Intrinsically disordered proteins (IDPs) are deeply involved in the pathogenesis of type 2 diabetes mellitus (T2DM) due to their flexible structures, which enable them to interact with multiple molecules and regulate key biological processes. Proteins such as IRS1, IRS2, and IRS4, which mediate insulin signaling, are highly disordered and play crucial roles in glucose metabolism. Their disordered regions often serve as hubs for protein-protein interactions and post-translational modifications, which are essential for proper insulin function. Dysregulation of these IDPs can impair signaling pathways, contributing to insulin resistance and hyperglycemia. Understanding the functional roles of IDPs in diabetes provides insights into novel therapeutic targets, potentially paving the way for innovative drug discovery aimed at stabilizing or modulating their activity. Using state-of-the-art computer simulations we will reveal structural details of IDPs involved in the pathogenesis of T2DM, identify temporary folds or binding sites, that might contribute to diabetes when disrupted. By understanding IDPs' dynamic behavior, researchers can design drugs that stabilize or block their harmful interactions—opening doors to treatments that were previously impossible to develop.	Students from chemical engineering, chemistry, physics, engineering physics, Biotech/BioEngineering. (Mathematics in Std. XII required) Specific skill set: interest in biomolecular modelling and simulations, interest in coding
Swati Bhattacharya	Computational study of Cancer Related Intrinsically Disordered Proteins: Insights for Understanding Disease Mechanisms and Guiding Therapeutic Discovery	SwB-TA or SwB-FA	Computational biophysics	Theoretical / Computational / Modelling	Intrinsically disordered proteins (IDPs) play critical roles in cancer by regulating cell cycle control, apoptosis, and signal transduction through highly flexible regions that can interact with multiple partners. Examples such as NUPR1, the N terminal domain of p53, and the transactivation domain of c Myc are central to oncogenic or tumor suppressive pathways and are increasingly viewed as promising drug targets. Molecular dynamics (MD) simulations allow us to study how these IDPs move, how mutations or post translational modifications alter their interactions, and where small molecules might bind to stabilize or disrupt their function. By combining MD with experimental data, we can identify key interaction sites and dynamic features that can be exploited for therapeutic discovery, paving the way for new strategies to target cancer related IDPs with precision drugs	Students from chemical engineering, chemistry, physics, engineering physics, Biotech/BioEngineering. (Mathematics in Std. XII required) Specific skill set: interest in biomolecular modelling and simulations, interest in coding

TA or FA topics

Bharatkumar Suthar	Development and Electrochemical Modeling of Low-Temperature Optimized Sodium-Ion Batteries	BKS-TA or BKS-FA	Batteries	Both: Theoretical (Computational or Modelling) + Experimental	This PhD project aims to develop low-temperature optimized sodium-ion batteries for reliable operation in demanding environments (0 to −20 °C), with relevance to defence and strategic applications. The work combines experimental development (materials, cell fabrication, and diagnostics) with physics-based electrochemical modeling to understand and overcome key limitations such as transport constraints, interfacial resistance, and performance degradation. The outcome will be robust battery designs and predictive tools for operation in cold and harsh conditions.	Chemical Engg/Physics/Electrochemical Engineering
Bharatkumar Suthar	Smart Diagnostics of Grid-Integrated Battery Systems Using Physics-Based Models and Machine Learning	BKS-TA	Batteries	Theoretical / Computational / Modelling	This project aims to understand how batteries used in grid applications degrade over time and how their performance drops under real operating conditions. It will combine simple physics-based models with machine learning to develop tools that can monitor battery health, detect early signs of degradation, and predict remaining life. The goal is to build reliable and practical methods that work with real-world data from grid operations such as renewable energy integration and peak load management. Preferred Background Basic understanding of batteries or electrochemistry Interest in modeling and data analysis Some experience with Python or machine learning	Chemical Engg/EE/Physics
Bharatkumar Suthar	Zinc-Ion Batteries for Affordable Grid Storage	BKS-TA	Batteries	Both: Theoretical (Computational or Modelling) + Experimental	Zinc-ion batteries (ZIBs) are emerging as a promising option for low-cost, large-scale grid storage, especially in the Indian context where affordability and material availability are critical. Based on abundant and non-critical materials like zinc and water-based electrolytes, ZIBs offer inherent safety and supply-chain resilience compared to lithium-ion systems. This research will focus on developing physics-based models and simulation tools to understand performance and degradation, and to guide scale-up from lab cells to practical grid systems. The goal is to enable robust, economical energy storage solutions tailored for renewable integration and decentralized power needs in India.	Chemical Engg/Physics
Sharad Bhartiya	Behavioral systems theory based MPC	SBh-TA	Control Theory	Theoretical / Computational / Modelling	Dynamics systems are usually represented by transport type equations. Behavioral systems are based on a representation-free approach where the system behavior is manifested in terms of dynamic trajectories. This work will explore data enabled predictive control (DeePC)	control theory, applied math, coding
Santosh Noronha	Production of chiral pharma intermediates	SN-TA or SN-FA	Genetic engineering	Experimental	The objective of this project is to overproduce a key chiral pharma intermediate, currently extracted from plants. The strategies we propose to use include transferring pathways to microbial systems from plants and other microbial systems, manipulation of pathway fluxes in these systems, and engineering relevant enzymes to have improved catalytic activities.	Project-related experience with biochemistry, microbiology and molecular biology techniques would be an advantage.
Santosh Noronha	Catalytic bioreactors	SN-TA or SN-FA	Industrial Biotechnology	Experimental	"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."	Exposure to process reaction engineering or biocatalysis.

TA or FA topics

Abhijit Majumder	Placenta on Chip	AbM-TA or AbM-FA	Organ on chip, microfabrication and microfluidics, CFD	Both: Theoretical (Computational or Modelling) + Experimental	https://wyss.harvard.edu/media-post/introduction-to-organs-on-a-chip/ Organ on chip is the futuristic technology to be used in drug discovery. The project aims to develop a placenta on chip, to be used for toxicity testing. The work will involve microfabrication, microfluidics, cell biology, and computational techniques. Hence, we are looking for a candidate who doesn't hesitate to step outside their comfort zone.	
Arindam Sarkar	High-capacity Prussian blue cathodes for Zn ion battery	AS-TA or AS-FA	Electrochemistry	Experimental	Recent investigations in my laboratory suggest that Prussian Blue, particularly copper Prussian Blue analogues, can serve as effective cathode hosts for a dual ion–zinc battery system. These materials are attractive due to their open framework structure, tunable composition, and ability to accommodate multivalent ions, making them promising candidates for next-generation energy storage devices. The proposed work will build on these findings by systematically exploring Prussian Blue and its analogues to further enhance electrochemical performance, particularly with respect to capacity and cycling stability. A key focus of the study will be understanding the role of structural water content, which appears to be a critical parameter influencing ion transport and, consequently, electrode performance. The project will involve the synthesis of Prussian Blue materials under varying conditions, followed by detailed characterisation to identify the factors governing water incorporation and structural stability. These materials will then be evaluated as cathodes through battery fabrication and electrochemical testing. Overall, the work aims to establish structure–property relationships that can guide the design of high-capacity, stable electrodes for zinc ion battery systems. Students undertaking this project are not expected to have prior experience in electrochemistry, as the necessary background and training will be provided during the course of the project. (1) Palacios-Corella, M.; Echevarria, I.; Santana Santos, C.; Schuhmann, W.; Ventosa, E.; Ibáñez, M. Prussian Blue Analogues as Anode Materials for Battery Applications: Complexities and Horizons. Chem. Mater. 2025, 37 (12), 4203–4226. https://doi.org/10.1021/acs.chemmater.5c00213. (2) Li, Y.; Zhao, J.; Hu, Q.; Hao, T.; Cao, H.; Huang, X.; Liu, Y.; Zhang, Y.; Lin, D.; Tang, Y.; Cai, Y. Prussian Blue Analogs Cathodes for Aqueous Zinc Ion Batteries. Materials Today Energy 2022, 29, 101095. https://doi.org/10.1016/j.mtener.2022.101095.	

TA or FA topics

Arindam Sarkar	All-iron redox flow battery	AS-TA or AS-FA	Electrochemistry	Experimental	The project will focus on the development of an all-iron redox flow battery, particularly employing non-aqueous electrolytes. Although all-vanadium redox flow batteries (VRFBs) have been successfully developed and commercialized, their widespread deployment is constrained by resource availability and cost, especially in the Indian context. In this regard, iron-based redox flow batteries present a promising and more sustainable alternative. However, several challenges remain for iron-based systems. One of the most significant limitations is the low plating efficiency of iron in aqueous media, which adversely affects performance and cycling stability. Recent work in our laboratory has explored the use of non-aqueous electrolytes, where improved plating behavior has been observed. This opens up a viable pathway for leveraging the multiple oxidation states of iron to design an efficient and stable redox flow battery system. The project will primarily involve experimental investigations, complemented by basic modelling efforts, aimed at developing a practical and efficient all-iron redox flow battery. Importantly, students undertaking this project are not expected to have prior experience in electrochemistry, as the necessary background will be developed during the course of the work. (1) Anwar, M. S.; Sarkar, A. Iron-Tungsten Redox Flow Battery. J. Electrochem. Soc. 2021, 168 (10), 100540. https://doi.org/10.1149/1945-7111/ac3160. (2) Hruska, L. W.; Savinell, R. F. Investigation of Factors Affecting Performance of the Iron-Redox Battery. J. Electrochem. Soc. 1981, 128 (1), 18–25. https://doi.org/10.1149/1.2127366.	

TA or FA topics

Arindam Sarkar	Investigating the Underlying Unity of Chemical and Electrochemical Processes	AS-TA or AS-FA	Catalysis	Experimental	It has been reasonably established that catalytic chemical oxidation and electrochemical oxidation are not fundamentally different or unrelated processes. Rather, they appear to be different manifestations of the same underlying electrochemical mechanism. In this context, the project aims to develop a more unified framework for comparing chemical and electrochemical oxidation pathways, building on the work conducted by previous students. The selected candidate will be expected to extend this research and rigorously investigate the equivalence between chemical and electrochemical oxidation mechanisms, particularly in non-aqueous systems. A key focus will be on understanding the role of dopants and poisons in modulating these pathways. At a later stage, the project may also involve the synthesis of nanoparticulate catalysts. While prior experience in electrochemistry is not mandatory, the student should possess a strong interest in analytical electrochemistry and detailed analysis of current–voltage behavior and reaction mechanisms. The project is experimental in nature with a small degree of modelling. (1) Chauhan, N. L.; Dameera, V.; Juvekar, V. A.; Mahajani, S. M.; Suresh, A. K.; Sarkar, A. Correlation of Chemical and Electrochemical Catalysis-Importance of Half Reactions: The Case of Catalytic Oxidation of Ferrous Sulfate by Molecular Oxygen. Journal of The Electrochemical Society 2018, 165 (5), H196–H204. (2) Chauhan, N. L.; Juvekar, V. A.; Sarkar, A. Oxidation of Ethylene Glycol: Unity of Chemical and Electrochemical Catalysis. Electrochemical Science Advances 2022, 2 (6), e2100092.	

TA or FA topics

Arindam Sarkar	Investigations on electrochemical CO2 reduction to formate/other C1/C2 chemicals	AS-TA or AS-FA	ECO2RR	Experimental	This is an experimental research project centered on the electrochemical reduction of carbon dioxide (CO_2) into formate or other high-value chemical products (1,2). The work will explore the design, synthesis, and application of metal and alloy-based catalysts, with a particular emphasis on their integration into gas diffusion electrodes (GDEs). One of the features would be to investigate the effect of gas composition on the products. These catalyst coated electrodes will be tested and optimized within a novel electrochemical setup, primarily utilizing a two-electrode flow cell configuration, although a three-electrode system may also be employed for more detailed mechanistic studies. The experimental tasks will involve the synthesis of nanoparticles and catalytic materials, followed by comprehensive physico-chemical and electrochemical characterization. Techniques may include, but are not limited to, transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry (CV). The products will be analyzed using HPLC/GC. Although prior experience in electrochemistry is not a prerequisite, the student is expected to develop a strong foundation in advanced electroanalytical techniques and physical characterization methods over the course of the project. This experience will be integral to understanding catalyst performance and reaction mechanisms in CO_2 electroreduction systems. The project is experimental in nature. Al-Tamreh, S. A.; Ibrahim, M. H.; El-Naas, M. H.; Vaes, J.; Pant, D.; Benamor, A.; Amhamed, A. Electroreduction of Carbon Dioxide into Formate: A Comprehensive Review. ChemElectroChem 2021, 8 (17), 3207–3220. https://doi.org/10.1002/celc.202100438. Giri, S. D.; Mahajani, S. M.; Suresh, A. K.; Sarkar, A. Electrochemical Reduction of CO2 on Activated Copper: Influence of Surface Area. Materials Research Bulletin 2020, 123, 110702. https://doi.org/10.1016/j.materresbull.2019.110702.	
P Sunthar	Optimizing Lithium-Ion Battery Cycles for Maximised Lifetime and Safety	PS-TA or PS-FA	Batteries	Theoretical / Computational / Modelling	"The performance and lifespan of Lithium Ion Batteries (LIBs are limited by the irreversible degradation in a battery cell. This project aims to understand the processes at the cell level to obtain optimal charging and discharging protocols for various load demands and renewable energy production rates. We will employ tools such as Discrete Element Method (DEM) and physics-assisted machine learning (PAML) and physics-informed neural networks (PINN) in an attempt to solve the problem.	Chemical Engineering, Physics, Python
Amol Subhedar	Lattice Boltzmann Modeling of Rarefied Flows in Complex Porous Geometries	AmS-TA	CFD/lattice Boltzmann	Theoretical / Computational / Modelling	The goal is to develop a general lattice Boltzmann model for high (~10^{-3}) Knudsen numbers flow in porous media. The challenges involve maintaining numerical stability at high Knudsen numbers in complex geometries. Focus will be on specular boundary conditions. The project involves developing and testing a model with C++/Python code.	Engineering background with strong programming skills
Jhumpa Adhikari	Phase change materials for carbon capture	JA-TA or JA-FA	Thermodynamics and Molecular Simulations	Theoretical / Computational / Modelling		Chemical Engineering, Interest in coding

TA or FA topics

Pramod Wangikar	Computational Analysis of mass spectrometry Data for mRNA Characterization	PW-TA or PW-FA	bioinformatics	Theoretical / Computational / Modelling	Mass spectrometry provides a rich but underutilized signal for characterizing long RNA molecules, where challenges include incomplete fragmentation, ambiguous sequence mapping, and detection of nucleotide modifications. This project will focus on developing computational methods and algorithms for the analysis of LC–MS/MS data from mRNA. Key objectives include sequence reconstruction from partial fragment information, detection and localization of chemical modifications, and statistical scoring of candidate structures. The work will involve modeling fragmentation patterns, designing efficient search or alignment strategies, and handling uncertainty arising from noisy and incomplete data. The developed methods will be applied to study mRNA degradation patterns and structural variability, with the goal of linking observed mass spectrometric features to underlying sequence and modification states. The outcome will be a set of scalable computational tools and models for high-confidence interpretation of MS data for large RNA systems.	Background in data science and knowledge of coding.
Pramod Wangikar	Computational Analysis of MS Data for Synthetic Peptide Characterization	PW-TA or PW-FA	bioinformatics	Theoretical / Computational / Modelling	Mass spectrometry is widely used for characterization of synthetic peptides, but analysis remains challenging due to sequence variants, side products, and the presence of non-canonical (unnatural) amino acids. Unlike proteomics, where sequences are drawn from known databases, synthetic peptide workflows require identification of expected products alongside a diverse set of impurities and intermediates generated during synthesis. This project will focus on developing computational methods and algorithms for interpretation of LC–MS/MS data from synthetic peptide systems. Key challenges include identification of truncated or modified sequences, detection of synthesis-related impurities (e.g., deletions, insertions, protecting-group remnants), and handling of non-standard amino acids with unknown or variable fragmentation behavior. The work will involve designing flexible sequence representation and search strategies, modeling fragmentation patterns for both canonical and unnatural residues, and developing scoring frameworks to distinguish closely related peptide variants. Efficient handling of combinatorial impurity space and uncertainty in spectral interpretation will be central to the approach. The developed methods will be applied to characterize peptide synthesis pathways, identify dominant impurity classes, and reconstruct intermediate species from MS data. The outcome will be a set of scalable computational tools and models for high-confidence interpretation of MS data in synthetic peptide systems, with emphasis on algorithmic robustness to sequence variability and chemical diversity.	Background in data science and coding experience

TA or FA topics

Rochish Madhukar Thaokar	Development of theoretical tools for droplet and cell electrohydrodynamics	RT-TA or RT-FA	Fluid Mechanics	Theoretical / Computational / Modelling	The project aims at developing a comprehensive model, currently lacking in the literature, for simultaneous electroporation and electrodeformation in vesicles and excitable (such as Neurons and Cardiomyotcytes) and non-excitable nucleate and anucleate cells, relevant in electroporation for cancer treatment. On the other specturm it will also be extended to droplet electrohydrodynamics relevant in crude oil refining. The simulatino platform will be in-house Boundary Integral code, as well as COMSOL Multiphysics and other open source softwares. T	Engineering, Chemical, Mechanical
Jyoti Seth	Why Do Like-Charged Polymers Stick Together?	JS-TA or JS-FA	Self-Assembly	Theoretical / Computational / Modelling	Normally, materials with the same charge repel each other. But in some cases, such as with the polymer polyethylenimine (PEI) in acidic water, chains can come together to form fascinating structures. This PhD project will use computer simulations (and possibly some experiments) to determine why this happens. Some initial insights can be seen in these publications: https://doi.org/10.1021/acs.macromol.4c02207, https://doi.org/10.1021/acs.macromol.0c01501). The PhD work will train you on fundamentals of charged polymers, soft matter, self-assembly, mean-field modelling, molecular simulations.	Chemical Engg/Metallurgical Engineering/Chemistry/Physics
Jyoti Seth	Electrorheology of Networked Suspensions	JS-TA or JS-FA	Electrorheology	Both: Theoretical (Computational or Modelling) + Experimental	This PhD project will build on previous research demonstrating that electric fields can effectively break down particle networks, converting solid-like materials into low-viscosity liquids that flow easily. Previous publications can be seen here: https://doi.org/10.1039/d0sm01404d, https://doi.org/10.1063/5.0243962. Apart from furthering our understanding of these systems, one of the applications and end-goals is to create a cost-effective, reliable, and environmentally friendly method to prevent and clear wax blockages, improving oil flow while reducing operational disruptions and energy consumption.	Chemical Engg / Mechanical Engg / Metallurgical Engg / Physics / Chemistry / Materials Science
Jyoti Seth	Simulating the Elasticity of Soft Materials for Biomedical and Environmental Applications	JS-TA or JS-FA	Suspensions	Theoretical / Computational / Modelling	This PhD project will explore how the size, shape, and connectivity of nanoparticles or microparticles influence the strength, flexibility, and performance of materials such as tissue engineering scaffolds, clays, hydrogels, and oleogels. By using advanced computer simulations, we will analyze how these particles interact to form networks, how their connectivity impacts material properties, and how the networks respond under stress. A few experiments may also be performed to validate and complement the simulation results. The aim is to develop a predictive tool that enables the design of materials with optimal strength, flexibility, and network connectivity. This research will be valuable for industries ranging from biomedical engineering (e.g., tissue scaffolds), pharmaceuticals (e.g., drug delivery systems), materials science (e.g., hydrogels and oleogels for various applications), and environmental engineering (e.g., clay-based filtration materials).	Chemical Engg/Mechanical Engg/Physics/Chemistry/Material Science/Metallurgy/Civil Engg
Sujit Jogwar	Sustainable power production through biogas	SSJ-TA	Process Systems Engineering	Theoretical / Computational / Modelling	- Implement material and energy integration in integrated biogas-fuel cell-battery storage system for power production - Pursue optimal design using superstructure optimization - Design advanced control strategy to handle operational challenges	Chemical/Electrochemical Engineering background is preferred. Exposure to numerically solving ODE/PDEs is preferred.

TA or FA topics

Sujit Jogwar	Decarbonization through electrification	SSJ-TA	Process Systems Engineering	Theoretical / Computational / Modelling	1. Analyze the impact of electrification on optimal design and operation of chemical systems. 2. Pursue electrification of conventional systems via direct/indirect modes. 3. Address optimal design and control challenge associated with electrification.	Chemical/Electrochemical Engineering background is preferred.
Sujit Jogwar	Distributed control of interacting systems	SSJ-TA	Process Systems Engineering	Both: Theoretical (Computational or Modelling) + Experimental	1. Develop graph-theoretical contributions for synthesizing distributed architectures for advanced control 2. Validate the architectures via dynamic simulations 3. Experimentally verify and validate the theoretical contributions on benchmark systems like quadruple tank system.	Chemical/Instrumentation/Electrical/Control Engineering background is preferred. Exposure to numerical solution of ODEs is preferred.
Jason R. Picardo	Flow and mass transfer in the lungs and gut	JP-TA	Biofluid mechanics, multiscale modelling, , data-driven methods	Theoretical / Computational / Modelling	This project will address problems involving fluid flow and mass transfer in the human body, specifically in the lungs and gut. We are interested in using mathematical models to understand how inhaled particles (allergens, pathogens, drugs) mix and spread through the lung airways, how nutrients are taken up by the intestines, and other similar biomedical problems. These questions require a multi scale modelling approach to deal with the wide range of spatial and temporal scales across which flows occur in the human body. An important technique in this context is reduced order modelling via rational methods from dynamical systems theory, as well as data-driven strategies. Webpage: https://sites.google.com/view/jrpicardo	To enjoy working on this problem you must seriously want to learn, understand, and apply techniques of multi scale modelling and simulation. By year 2 of your PhD, you will have to be strong in fluid dynamics, theory of ODEs and PDEs, and numerical methods. So a good foundation in these subjects will help. A lot of reading, especially of biomedical literature, will be needed to frame the problems and develop the model.
Jason R. Picardo	Patterns in turbulence: emergence of order amidst chaos	JP-TA	Stochastic dynamical systems, turbulence, pattern formation	Theoretical / Computational / Modelling	The vast majority of flows in our daily experience are turbulent and yet we see patterns all around us. Ordered arrays of cloud streets, (turbulent) wind-driven waves with distinct wavelengths, and---for a more exotic example---Jupiter's red spot all testify to the ability of ordered patterns to arise and persist amidst turbulent fluctuations. How such large scale patterns emerge and persist is a fundamental open question; from a practical perspective, one would like to know how turbulent fluctuations affect the large-scale patterns. Our approach in this project will be to model turbulence as a stochastic forcing and use methods from reduced order modelling and stochastic dynamical systems to answer the above questions. The specific problems we will tackle have applications in weather/climate, human lungs, catalytic converters, etc. Webpage: https://sites.google.com/view/jrpicardo	To enjoy working on this topic you must seriously want to learn, understand, and apply theories of pattern formation, stability analysis, and stochastic dynamics. By year 2 of your PhD, you should be strong in fluid dynamics, mathematics of ODEs and PDEs, and numerical methods. So a good foundation in at least some of these topics will be very helpful.

TA or FA topics

Rajdip Bandyopadhyaya	Chemical sensor device development for detection of water pollutants and technology for their removal	RB-TA or RB-FA	Water treatment	Experimental	We have already developed in our lab. an autonomous device for real-time, water quality monitoring by both physical and chemical sensors (some of the sensors being developed by us), with years of earllier work in our lab. by a multidisciplinary team. We have also worked extensively on separation and removal of pollutants (arsenic, heavy metal, fluroride etc.) from water, by our nanoparticles and composites. In this PhD project now, we will combine above steps of sensing and removal of pollutants from water. For this, first we will combine both physical and chemical sensors in a single device. Next, reactive adsorption of these pollutants by nanoparticle coated polymereic fibre will be carried out, to provide clean drinking water. Thus one has to have either some background or interest in chemical, environmental, materials engg. for basic research or have liking of designing and fabricating of electromechanical devices, to fit into our current team and carry out PhD research.	Engineering (Chemical, Environmental, Mechanical, Electrical) or Science (Chemistry, Materials, Nanoscience)
Rajdip Bandyopadhyaya	Gravity-driven device for removal of microorganisms, metals and microplastics from water	RB-TA or RB-FA	Water treatment	Both: Theoretical (Computational or Modelling) + Experimental	We have already developed a working prototype for killing and removal of E. coli from water. It is based on our synthesized nanocomposite, made of Ag-Cu nanoparticle impregnated on granular activated carbon and packed into a column, which is driven by gravity-head of the water column. Consequently, it can continuously disinfect water in absence of electricity, by the action of nanoparticles on the bacteria. In the current project, the aim is to further study the removal of heavy metals and microplastics, by the same or related class of nanocomposites, as these are all critical contaminants present in water. The final outcome would be a modular water treatment device, usable for household drinking water needs, by combining concepts of adsorption, reaction engineering, fluid flow and functional design principles to make a energy self-sufficient device. The work is mostly experimental with reasonable scope of modeling, if the student is interested. They get to work and learn in a multidisciplinary team of bio-sciences and engineering students, contributing to the overall goal of the project. One has to have background in either engineering/design/modeling disciplines or inn microbiology/biology/chemistry; but not both exposure are needed. Thus one can do only experiment or a combination of experiment and modeling.	Engineering (Chemical, Environmental, Mechanical) or Sciences (Chemistry, Microbiology, Materials, Nanotech., Biological)

TA or FA topics

Rajdip Bandyopadhyaya	Engineering nanoparticle size and shape: multiscale modeling, simulation and applications	RB-TA or RB-FA	Nanoparticles	Both: Theoretical (Computational or Modelling) + Experimental	Nanoparticles show new and interesting properties different from bulk materials due to their extremely small size (diameter), large specific surface area and spatial anisotropy. It is thus critical to understand the variables that control its synthesis, leading to a desired application. Control of mean nanoparticle size, particle size distribution and specially, anisotropic particle shapes is the first step in many of these applications, involving enhanced adsorption and reaction rates. To gain further insight into the mechanism of formation of nanoparticles, we have already developed models on how individual nanoparticles form by processes like multiphase mass transfer, reaction, nucleation, Brownian collision, surface growth, coagulation and Ostwald ripening, followed by interparticle forces and differential growth rates along different crystal facets, leading to anisotropic particles. With the above mechanism in place, in this PhD project, one has to build on our existing mesoscale mathematical models (population balance equations) and computer simulation (kinetic Monte Carlo) codes to apply for nanoparticle formation and growth in microemulsions, macroemulsions and bulk solvents. In conjunction, one can also carry out experiments, if required, involving other complex nanostructures, like core-shell or oval and flower-shaped nanoparticles, besides cylindrical nanorods. Copper/silver/gold as metallic and iron oxide/zinc oxide/silica as metal oxide nanoparticles will be considered as typical model systems, since we are already using them, for different applications, like, chemical sensing, water purification devices, catalysis and drug delivery. Thus, the student can only perform multiscale computational research (using population balance equation or kinetic Monte Carlo simulation) or do a combination of experiments and modeling. Depending on the student's interest, there would be further scope to use the model and simulation predictions with available or new experimental data, for improving these exciting applications of nanotechnology. Finally, exploring whether anisotropic particles can display enhanced reactivity, is of paramount importance, as it will open up a new paradigm in reaction engineering. This will lead to enhancement in rates of existing or new chemical reactions, utilizing such particles as catalysts. It can be a potential new paradigm in reaction engineering.	Engineering (Chemical, Mechanical, Materials) or Science (Physics, Chemistry, Nanotech.)
Mani Bhushan and Ravi Gudi	Digital twin based decision support system for process design and operations	MB-TA	Process Systems Engineering	Theoretical / Computational / Modelling	Digital twin is a model of a physical system that should mimic the system at all times. To be able to mirror the system, it should incorporate physics knowledge- represented as constraints, regularization, or structure, as well as measurements from the plant in real-time. This work will investigate various optimization, and control-theoretic approaches for the same, thereby enabling a decision support system for taking design and operational decisions based on the predictions from digital twins.	Interest in Maths, Probability/Statistics and Coding

TA or FA topics

Partha Sarathi Goswami and Devang Khakhar	Rheology and dynamics of dense, turbulent fluid-solid flows	PSG-TA or PGS-FA	Fluid Mechanics/Suspensions	Both: Theoretical (Computational or Modelling) + Experimental	Turbulent, dense fluid-particle flows are commonly encountered in engineering and natural process, transport of suspensions in chemical and pharmaceutical industries, bed load 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. Most of the studies, reported in the literature have focused either dilute phase turbulent flows or dense phase solid system with laminar flows. The primary objective of the present work is to build a better fundamental understanding of the dynamics and the rheological behavior of the turbulent fluid-solid systems using interface resolved-direct numerical simulation and experiments.	Chemical Engg/Mechanical Engg/Physics
Partha Sarathi Goswami and Devang Khakhar	Theoretical and experimental studies on segregation behaviour of cohesive and non-cohesive powders under vertical transport	PSG-TA or PGS-FA	Fluid Mechanics/Granular flows	Both: Theoretical (Computational or Modelling) + Experimental	Powder handling and transport are vital operations in the pharmaceutical industry. Vertical transfer of powders often leads to segregation due to differences in particle size, density, and cohesion, which adversely affect the product uniformity and follow-up processes. Specific objectives of the present projects are Determination of segregation as a function of particle size ratio and air flow conditions using high-speed imaging, quantification of segregation behavior of cohesive and non-cohesive powders during vertical flow under air-present and air-absent conditions, and correlating segregation behavior with air pressure and flow rate using synchronized sensors and visualization tools.	
Partha Sarathi Goswami	Nonisothermal particle laden turbulent flows: direct numerical simulations (DNS) and experiments	PSG-TA or PGS-FA	Turbulence	Both: Theoretical (Computational or Modelling) + Experimental	Particle laden turbulent flows are encountered in many natural and industrial processes, e.g., pneumatic transport of solids, spray combustion, particle-based solar receivers, pollutant dispersion in urban areas, spray drying etc. In such flows, there is a strong coupling between the solid and fluid phases, which determines the simultaneous dynamics and multiphase transport processes. Heating of the particles by external heat source like radiation, chemical reaction etc, can introduce temperature fluctuation and generate local fluid fluctuation. Non uniform distribution of the particles will introduce more inhomogenity in the intensity of turbulence which may further influence particle distribution. The present project aims to quantify the effect of particle temperature of the fluid phase turbulence and model the macroscopic transport rate with the particle scale information.	Chemical Engg/Mechanical Engg/Physics
Hemant Nanavati	Accurate Molecular Models for Real Polymers	HN-TA or HN-FA	Polymer Chemical Physics	Theoretical / Computational / Modelling	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.	(Chemical Engg/Chemistry/Physics/Materials Science/Polymers) + Knowledge of coding
Hemant Nanavati	Molecular Modeling of Elasticity of Spider Silk and Related Biopolymers	HN-TA or HN-FA	Biopolymer Physics	Both: Theoretical (Computational or Modelling) + Experimental	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.	(Chemical Engg/Chemistry/Physics/Materials Science/Polymers) + Knowledge in coding

TA or FA topics

Sameer Jadhav	Simulation-Based Characterization of Mass Transport and Reaction Dynamics in Enzymatic Microreactors	SRJ-TA or SRJ-FA	Biofluid mechanics	Theoretical / Computational / Modelling	This project utilizes the open-source CFD platform OpenFOAM to develop a generalized computational framework for simulating biocatalytic processes within wall-coated microreactors. By integrating the Navier-Stokes equations with scalar transport models, the simulation captures the complex interplay between laminar flow hydrodynamics and surface-bound Michaelis–Menten kinetics, implemented as a custom boundary condition. Through a parametric analysis of dimensionless transport numbers, the model identifies the critical transitions between diffusion-limited and reaction-limited regimes, allowing for the optimization of reactor geometry and flow rates. Ultimately, this research provides a scalable, in-silico tool for predicting conversion efficiency and maximizing biocatalyst productivity across diverse industrial applications, ranging from green chemistry synthesis to high-throughput pharmaceutical screening.	B.Tech/M.Tech in Chemical Engineering, Mechanical Engineering, Biotechnology
Yogendra Shastri	Sustainable Energy Transition Planning for India - Modeling and Analysis	YS-TA or YS-FA	Energy	Theoretical / Computational / Modelling	India is on a path of rapid socio-economic transformation and has set ambitious targets to increase the size of its economy. India has also committed to achieving net-zero status by 2070. To achieve this target, the energy sector has to lead the transition. This transition also needs to follow sustainability principles. The key objectives of this project are to address the following questions: - How can key sectors, such as power, oil and gas, and chemicals, plan the transition to net-zero? - Which technologies are likely to succeed and must be prioritized (e.g., green hydrogen, biofuels, e-fuels, etc.)? - What are the desirable and expected timelines for the adoption of these technologies? - How do the different transition pathways compare in terms of sustainability? This is completely computational work, and is quite interdisciplinary.	Chemical engineering (experience in computer modeling will be desirable but not necessary)
Yogendra Shastri	Bienergy system design considering food-energy-water-climate nexus	YS-TA or YS-FA	Bioenergy	Theoretical / Computational / Modelling	Bioenergy options, such as ethanol, compressed biogas (CBG), and biopower, are expected to play an important role in the future energy mix, considering their potential to mitigate greenhouse gas emissions. However, biomass resources are limited and seasonally available. Moreover, the availability of biomass is increasingly impacted by climate change. Therefore, it is essential to plan a biomass utilization strategy for bioenergy, considering these complexities. The objective of this project would be to use an optimization framework to answer these questions. The specific objectives are: 1. Quantify the impact of climate change on biomass availability 2. Develop models (possibly based on AI/ML) to assess biomass availability as a function of climate change. 3. Develop an optimization model to strategize biomass utilization among various sectors. 4. Provide technology and policy recommendations for the bioenergy sector. The work is computational in nature and interdisciplinary. It will involve developing optimization models and collecting data for various sources.	Chemical Engineering, Operations Research, Industrial Engineering, Environmental Engineering

TA or FA topics

Yogendra Shastri	Development of an open-source tool for life cycle assessment of transport sector	YS-TA or YS-FA	Sustainability	Theoretical / Computational / Modelling	Life cycle assessment has become a very important tool to assess the environmental impact of technologies are products. For the transport sector, many new options, such as battery operated EVs, CBG vehicles, and fuel cell vehicles are being developed. These vehicles may penetrate and take up a large share of vehicles in India. However, India currently lacks a comprehensive tool to perform life cycle assessment (LCA) of these options. India a need a tool like GREET (https://www.energy.gov/cmei/greet) for providing details in the Indian context. The goal of this project is to address this gap. The specific objectives are: 1. Perform LCA of key technologies in transport sector for India. 2. Develop a generic GREET like framework for India. 3. Incorporate open source information and research results into the LCA model. 4. Refine the model into a decision support tool. This is a very applied work and will be interdisciplinary. The application of this tool is in policy-making and technology benchmarking.	Chemical engineering, Environmental engineering