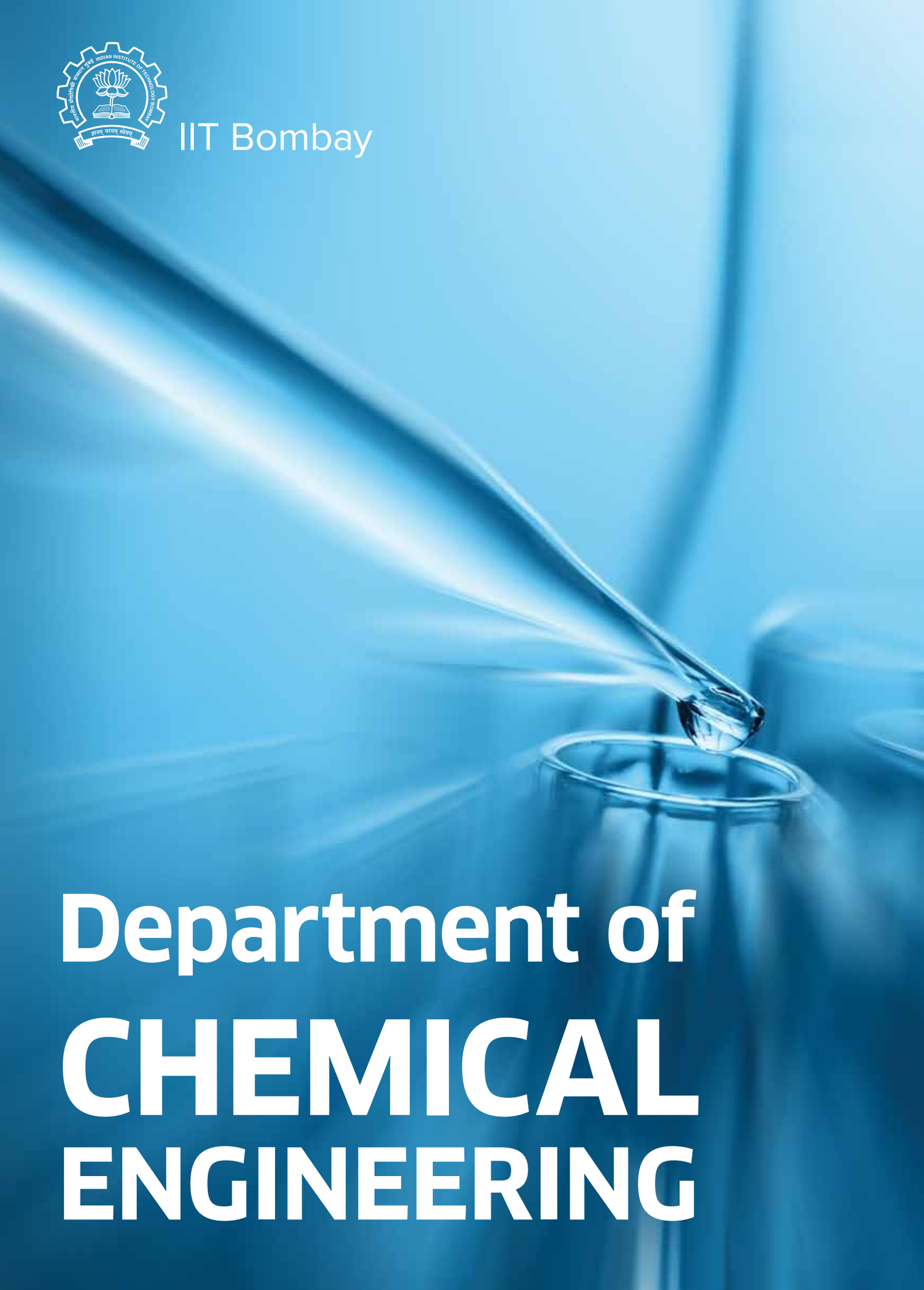


IIT Bombay

Department of CHEMICAL ENGINEERING

Department of
CHEMICAL
ENGINEERING

IIT Bombay

Department of Chemical Engineering

IIT Bombay, Powai, Mumbai - 400 076, India

Contents

The **Vision** of IIT Bombay is to be the fountainhead of new ideas and of innovators in technology and science.

It's **Mission** is to create an ambience in which new ideas and creativity flourish and from which research and scholarship and leaders and innovators of tomorrow emerge.

Photograph: Prashant Sharma

IIT Bombay

Established in 1958, the second of its kind, Indian Institute of Technology Bombay was the first IIT to be set up with financial assistance from the then Soviet Union. In 1961 Parliament decreed the IITs as 'Institutes of National Importance'. Since then, IITB has grown from strength to strength to emerge as one of the top technical universities in the world.

The institute is recognised worldwide as a leader in the field of engineering education and research. Reputed for the outstanding calibre of students graduating from its undergraduate and postgraduate programmes, the institute attracts the best students from the country for its bachelor's, master's and doctoral programmes. Research and academic programmes at IIT Bombay are driven by an outstanding faculty, many of whom are reputed for their research contributions internationally.

IIT Bombay also builds links with peer universities and institutes, both at the national and the international levels, to enhance research and enrich its educational programmes. The alumni have distinguished themselves through their achievements in and contributions to industry, academics, research, business, government and social domains. The institute continues to work closely with the alumni to enhance its activities through interactions in academic and research programmes as well as to mobilise financial support.

Over the years, the institute has created a niche for its innovative short-term courses through continuing education and distance education programmes. Members of the faculty of the institute have won many prestigious awards and recognitions, including the Shanti Swaroop Bhatnagar and Padma awards.

Located in Powai, one of the northern suburbs of Mumbai, the residents of the institute reap the advantage of being in the busy financial capital of India, while at the same time enjoying the serenity of a campus known for its natural beauty. A fully residential institute, all its students are accommodated in its 18 hostels with in-house dining; the campus also provides excellent amenities for sports and other recreational facilities.

Message from Head of the Department

Welcome to the Department of Chemical Engineering at IIT Bombay. The department has a rich legacy of innovation and creativity in teaching and research for the past 57 years, which is as old as the Institute. We have excellent faculty with a rich experience in research and teaching in the broad areas of chemical engineering. We are proud of our alumni who have excelled in the profession by being leaders, thereby contributing to industry and academia. Our department has evolved as a place for research and technology development in the key areas of health, energy, environment and materials.

Academic programmes in our department include both under-graduate (Bachelor of Technology) and postgraduate degrees (Master of Technology and Doctor of Philosophy), with strong emphasis on chemical engineering principles along with application towards designing, optimizing and operating industrial processes. The research in the department is multi-disciplinary and contemporary including areas such as Biological Systems Engineering, Soft Matter Engineering, Process Systems Engineering, Catalysis and Reaction Engineering, Thermodynamics & Molecular Simulations and Energy, Environment & Sustainability, with a strong focus in the themes relating to healthcare, energy and materials.One of the main focus of the department is to produce exceptional future researchers in the field. Currently, the department has about 200 registered Ph.D students working in the above focus areas.

We have an active outreach programme through specialized small term courses for industry personnel in all aspects of chemical engineering. We have designed curriculum based on the requirement of specific industries for sponsored Masters programme. We also engage actively in R&D and consultancy projects with several leading industries of the country. In the coming years, the department looks forward to contributing towards fundamental and applied research, engaging with industry for technology development and train students to be leaders in chemical engineering profession.

Prof. K. V. Venkatesh
Head, Department of Chemical Engineering

Introduction to the Department

The Department of Chemical Engineering at IIT Bombay was established in 1958, which was made up of Chemistry and Industrial Chemistry Divisions. This was mainly due to the influence of USSR, which was supporting the institute then. In 1964, a separate Department of Chemistry was established, and thus Chemical Engineering evolved to form an independent department. Even today the two departments, Chemistry and Chemical Engineering are housed together in the same building. The department transformed post 1990s from having classical Chemical Engineering disciplines such as Transport, Reaction Engineering, Unit Operations, Petroleum, Electrochemical Engineering to include areas such as Systems Engineering, Biochemical Engineering, Polymer Engineering, Catalysis etc. In recent times, the flavour has further changed to include several scales from molecular to process to the plant. This has brought forth inclusion of modern biology, computational chemistry, complex fluids and nanomaterials into the academic stream of the department.

The Department of Chemical Engineering is one of the largest departments in the Institute in terms of faculty and student strength and research funds received. Currently, the department has 40 faculty, 14 post-doctoral candidates, 833 students (including 494 Bachelors, 119 Masters and 220 Doctoral), 25 supporting staff and 152 temporary project staff. The faculty strength has risen from 30 to 40 in the last five years with aggressive hiring in key emerging areas of chemical engineering to strengthen the existing focus of the department. The department has seen a steady increase in the strength of doctoral students resulting in a vibrant research culture. This is reflected in a large output in research as seen by publication record of the department (3.4 journal articles per faculty per year). The sponsored and consultancy projects funding is also increasing over the years with an average of about Rs. 75 lakh/faculty/year.. The diverse research areas of the department, including Biological Systems Engineering, Soft Matter Engineering, Process Systems Engineering, Catalysis and Reaction Engineering, Thermodynamics & Molecular Simulations and Energy, Environment & Sustainability, have a strong focus in the themes relating to healthcare, energy and materials. The breadth in these topics has resulted in courses in our curriculum as well as in the continuing education programme of the institute.

We currently offer degree programmes leading to Bachelor of Technology (B.Tech), Master of Technology (M.Tech and B.Tech + M.Tech dual degree) and Doctor of Philosophy (Ph.D and M.Tech + Ph.D dual degree). Over the years, the department has produced several distinguished alumni holding prominent positions in both industry and academia.

Heads of the Department

	NAME	FROM	TO
01.	**Prof. N. R. Kamath**	02/03/1959	01/07/1974
02.	**Prof. G. S. R. Narsimhamurthy**	01/07/1974	19/09/1977
03.	**Prof. S. K. Raman**	19/09/1977	09/12/1980
04.	**Prof. V. C. Rane**	09/12/1980	02/12/1983
05.	**Prof. K. P. Madhavan**	02/12/1983	02/02/1987
06.	**Prof. M. C. Dwivedi**	02/02/1987	01/02/1990
07.	**Prof.. S. L. Narayana Murthy**	01/02/1990	25/02/1993
08.	**Prof. M. K. Trivedi**	25/02/1993	29/02/1996
09.	**Prof. K. C. Khilar**	29/02/1996	22/04/1999
10.	**Prof. R. K. Malik**	22/04/1999	30/06/2002
11.	**Prof. D. V. Khakhar**	01/07/2002	10/01/2005
12.	**Prof. R. K. Malik**	10/01/2005	15/03/2005
13.	**Prof. A. K. Suresh**	15/03/2005	20.01.2008
14	**Prof. A. Mehra**	21/01/2008	21/01/2011
15.	**Prof. S. C. Patwardhan**	21/01/2011	18/11/2013
16.	**Prof. K. V. Venkatesh**	18/11/2013	Till Date

Academic Programmes

Bachelor of Technology (B.Tech)

The B.Tech program is a four-year course to which students are selected from a nationwide joint entrance exam (JEE). The strength has increased from 54 in 2008 to about 125 in 2015. As per the latest course curriculum, the students can opt for the M.Tech program in their third year and thereby earn a dual degree at the end of five years. The curriculum allows students to take a variety of elective courses that exposes them to the current trends of the profession.

Master of Technology (M.Tech)

The M.Tech program is a two-year course to which students are selected from a nationwide entrance exam (GATE). The current strength is about 65 (2015). The programme focuses on advanced topics in chemical engineering with sufficient credits allocated to project work. Almost all our M.Tech students are funded through MHRD (Ministry of Human Resources and Development) fellowships.

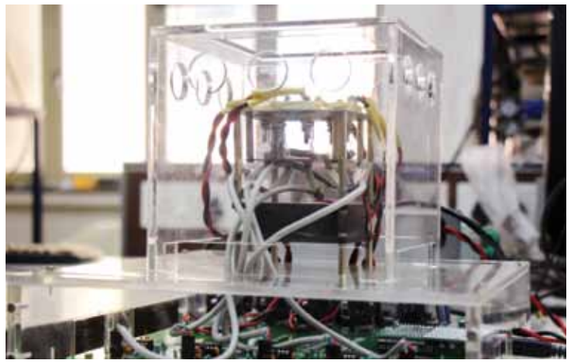
Doctor of Philosophy (Ph.D)

The department has a dynamic post-graduate programme with opportunities and strong emphasis on basic and applied research in a wide range of areas including several inter-disciplinary fields. This post-graduate programme includes a large number of Ph.D scholars who primarily contribute to the research activities of the department. The students can join the programme either with a Masters degree or a Bachelors degree in Engineering and Science. The selection is based on a written test and an interview. The number of students admitted to the Ph.D program has been averaging around 35 per year for the last five years (2011-2015). Almost all the students are funded with a fellowship of Rs 18,000-Rs 25,000/month in their first two years with higher amounts in the remaining three years (Rs 20,000-Rs 28,000/month). As part of the programme, the students are encouraged to present their research work in various national and international conferences. The institute provides funding to a tune of Rs 1.0 lakh for at least one international conference and more than one national conference. The department now accepts Ph.D applications throughout the year.

Areas of Research

The department has a vibrant research culture brought about by diverse and emerging areas that the faculty works on. The research environment in the department enables the students to work on diverse multi-disciplinary areas enhancing their ability to solve complex engineering problems. The research focus of the department can be divided into six groups, namely:

- Biological Systems Engineering
- Energy, Environment and Sustainability
- Thermodynamics and Molecular Simulations
- Soft Matter Engineering
- Catalysis and Reaction Engineering
- Process Systems Engineering



Research Themes

Biological Systems Engineering

- Biotechnology
- Systems and Synthetic Biology
- Metabolic Engineering
- Disease and Health
- Biomaterials
- Drug Delivery and Bio-Sensors
- Data Mining and Analysis
- Dynamics and Control

Energy, Environment and Sustainability

- Biomass and Biofuels
- Process Modeling and Energy Analysis
- Climate, Environment and Sustainability
- Fuel Cells
- Solar Thermal Power
- Combustion Systems
- Carbon Capture Systems

Thermodynamics and Molecular Simulations

- Materials
- Computer Methods
- Bio-inspired Systems

Soft Matter Engineering

- Colloids and Interface Engineering
- Granular and Particulate Flows
- Nano-structured Materials
- Drug Delivery
- Microfluidics

Catalysis and Reaction Engineering

- Catalysis
- Reactor Modeling
- Biofuels and Clean Coal Technologies
- Electrochemical Reactions and Fuel Cells
- Processing of Semiconductor Materials
- Multiphase Reactions

Process Systems Engineering

- Control Relevant Modeling
- Nonlinear Model Predictive Control
- On-line Fault Diagnosis and Fault Tolerant Control
- Nonlinear State Estimation
- Adaptive Control
- Flowsheet-wide Optimization
- Process Intensification

Biological Systems Engineering

Research in Biosystems Engineering is primarily focused on five themes, namely, (i) Disease and Health, (ii) Biomaterials, (iii) Development of Tools for Bioengineering, (iv) Bioenergy, and (v) Data/Systems Analysis. In the area of disease and health, our research focuses on understanding signaling pathways in cancer, whole body human metabolism towards disease characterization, cell culture engineering, study of cellular migration in responses to multiple cues, and antibiotic resistance and stress response in pathogens. In the area of biomaterials, the group has been focusing on development and characterization of nanostructured materials, their structure and their applications to health care and manufacturing processes. Particular areas of interest include: (a) micro-devices for cardiac use, (b) nano-composites for dental use, (c) drug delivery with nano-particles, (d) nanostructured hollow particles for dialysis, (e) stem-cell bioreactors and scaffolds, and (f) nanoparticles in alternate and traditional medicine. Work in the area of cell engineering and drug delivery focuses on measuring bio-membrane properties, liposomal drug delivery systems and stem cell expansion. A group of faculty are working towards development of tools to facilitate use of microorganisms as a platform for use as cell factories – these include design and characterization of cellular components to control transcription and translation. In the area of bioenergy, the group is working towards development of bacterial and algal strains and tools to yield high value chemicals and biofuels. Finally, in the area of Data/Systems Analysis, a group of faculty are working towards analysis and integration of large amounts of data generated from cells, and use a systems perspective to better understand the design principles employed by biological systems and organisms.

Energy, Environment and Sustainability

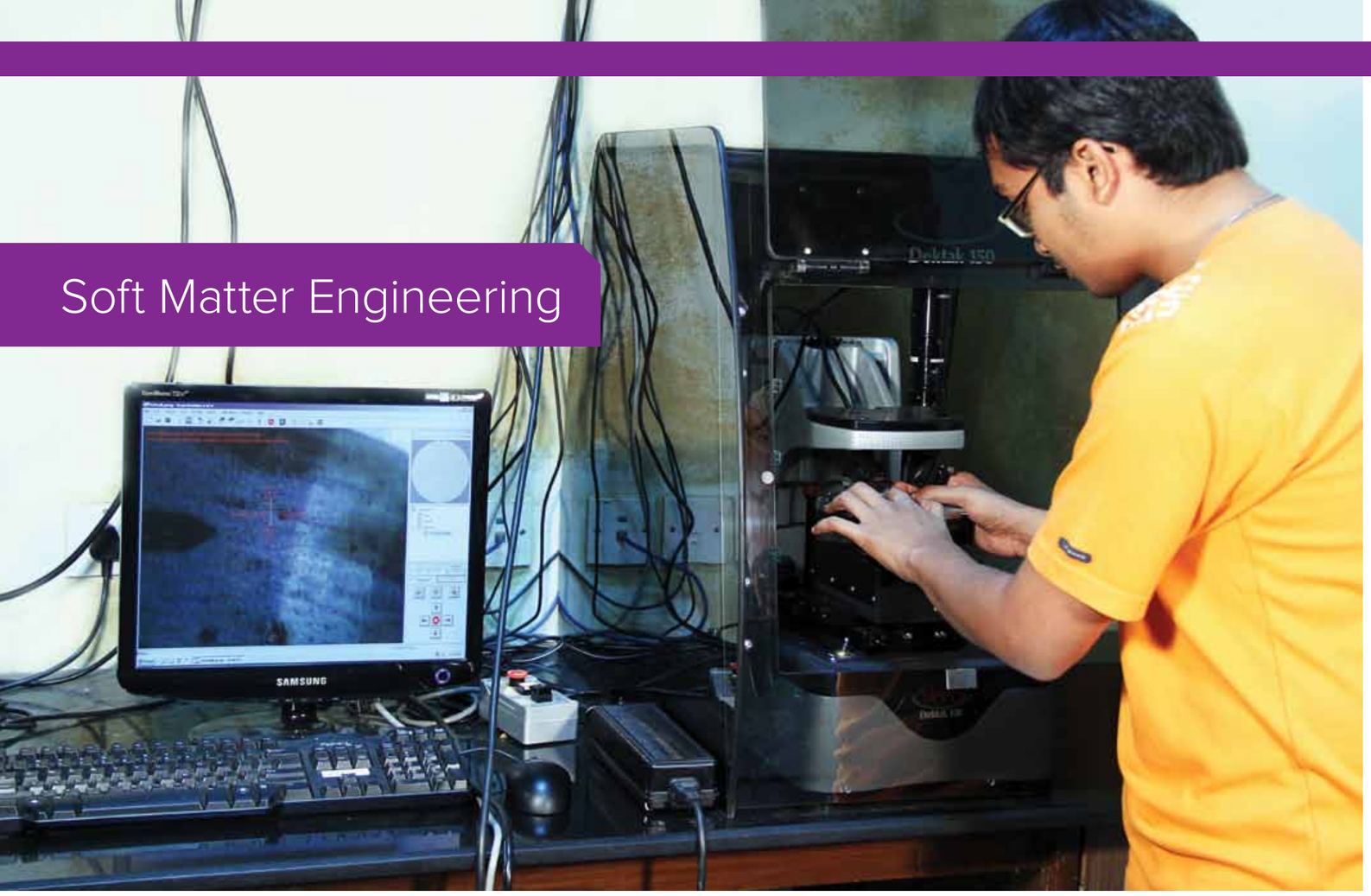
Ongoing research in the Energy, Environment and Sustainability area, addresses non-fossil energy, industrial energy, climate and environment. In the area of energy, major research topics under investigation are: Biomass and biofuels, Fuel cells, Solar thermal power, Process modeling and energy analysis and Combustion systems. In the area of biomass and biofuels, research addresses challenges at different scales. This includes work on improving biomass productivity through metabolic engineering, enhancing fuel production and selectivity through enzyme improvements, and achieving techno- economic feasibility through optimization approaches. In the area of fuel cells, research is aimed towards better selection of electrode materials by understanding processes that influence performance degradation. Work in the area of solar thermal power plants is focused in solving the challenging control problems in the domain. In industrial applications, work is mainly focused on industrial process modelling and energy integration as well as risk analysis. Research is also being carried out on in-situ coal gasification and biomass combustion under the theme of combustion systems.

In the broad and cross-cutting area of environment, which includes climate and sustainability, highly complex systems are being studied through phenomenological understanding and modeling of atmospheric constituents and transport, statistical methods for understanding and reducing uncertainty and complex systems-based modeling tools. The specific topics under investigation are: Climate, Sustainability, Water pollution, and Carbon capture systems.

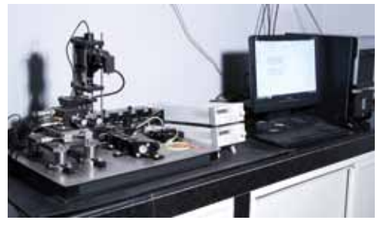
Thermodynamics and Molecular Simulations

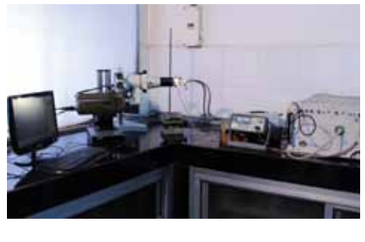
The research group working in the area of thermodynamics and molecular simulations study both hard matter, and soft matter systems, and have a wide variety of interests. Work carried on in the department is both applied and fundamental in nature. One of the areas of research pertains to the development of a multi-scale modeling scheme for compound semiconductors which find wide range of applications in the fabrication of opto-electronic devices. The group is also attempting to develop a computational scheme for rational solvent design for application to select the optimal solvent (or design a new solvent) for the extraction of a pharmaceutical intermediate synthesized using a biotransformation process. Novel multiscale simulation techniques are being developed which are motivated by the fact that reaction and diffusion mechanisms and their rate constants are still not well understood. These accelerated self- learning molecular models have addressed major challenges, namely, i) ability to find reaction and diffusion pathways and kinetic parameters spanning nanosecond to second timescales in a computationally feasible manner, ii) self-learning (automated) and computationally-parallelized techniques that can construct reaction networks on-the-fly, iii) machine-learning algorithms that predict the effect of local chemical bonding on the reaction kinetics, and iv) error estimates that ensure accurate prediction of materials evolution at experimental laboratory scales. The group also focuses on molecular simulations to understand, in detail, the interfacial phenomena and self-assembly process occurring in chemical systems. The research is focused towards design and synthesis of porous material, superhydrophobic surfaces and confined and interfacial fluids. Another area of research group pertains to the non-equilibrium dynamics of dense suspensions and nanostructured materials. The group's focus is on rheology and dynamics of dense colloidal suspensions that are of relevance to cosmetic, paint, pharmaceutical and petroleum industries. Research also focuses on the effect of anisotropies in the structure, phase behavior, and dynamics of soft condensed matter systems. Polymer nanocomposites, Pickering emulsions, soft-penetrable particles, and surface-corrugated colloids are current materials of interest.

Soft Matter Engineering

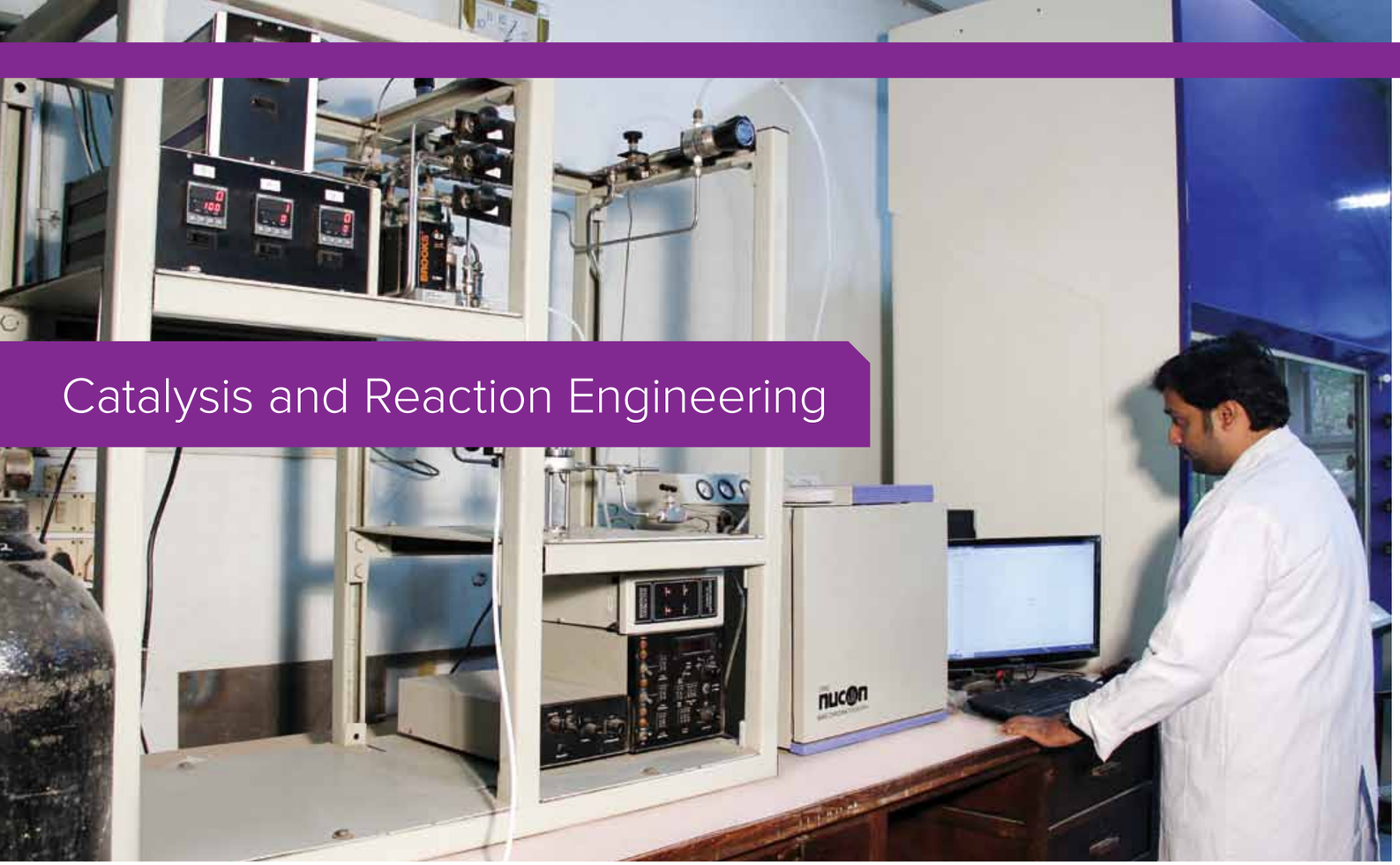


The soft matter engineering group pursues excellence in theoretical, computational and experimental expertise in synthesis, characterization and processing of soft matter. The group focuses on providing smart, holistic, engineering solutions to challenging problems in soft matter which fall under the two key areas of national interest, namely Energy and Environment and Health and Hygiene. The research problems can be further classified under the following five broad areas of chemical engineering, namely, (i) Hydrodynamics, Rheology and Granular Flows, (ii) Nano-structured Materials, (iii) Micro-fluidics and Micro-devices, (iv) Colloids and Interface Engineering, and (v) Electro-hydrodynamics. The general approach in the Soft Matter Engineering group has been to provide innovative solutions with an emphasis on fundamentals. The diverse expertise available in the department to address problems at microscopic, mesoscopic and continuum scales ensures a multi-scale understanding of any problem, a typical characteristic of soft matter. One of the major thrust areas of the soft matter engineering group is in synthesizing and developing new materials (biomaterials, composites, other soft materials) and uncovering the properties and applications of these materials, by investigating their structure and dynamics through experiments, theory and simulations. Specifically, under the broad area of Energy and Environment, the faculty of the soft matter research group focus on problems related to electro-emulsification, electro-spinning, electro-patterning, interplay of interfacial rheology and electric fields, tribology of soft interfaces, dynamics of charging/discharging process in conducting polymers, physics of film formation and cracking of paints and coatings, atomization processes applied to combustion, microfluidics as a tool for generation of polymer-based nanomaterials, dynamics of particle laden fluid flows, hydrodynamics of hydraulic jumps and cavitation, shear banding in amorphous solids, and development of molecular models to predict materials properties for catalysis and electronics applications. In the broad area of Health and Hygiene, the faculty are interested in problems related to development of aerogels for drug delivery from synthetic and natural materials, development of microfluidic devices for biological studies such as cell sorting and behavioral studies of microorganisms such as C. elegans, biophysics of bacterial locomotion, and physics of liposomes and elastic capsules. As the soft matter engineering group looks to the future, it aims to work on problems that are critical to the needs of the nation. These include design of hierarchically structured materials for carbon capture, energy storage, and water purification, suite of porous nanoparticle hosts for sensing, catalysis and drug delivery and mathematical models to address size and shape-controlled nanoparticle synthesis technologies for energy generation, harvesting and storage; and building lab-on chip technology for diagnostics and therapeutics and for sensing of trace molecules in air and water.





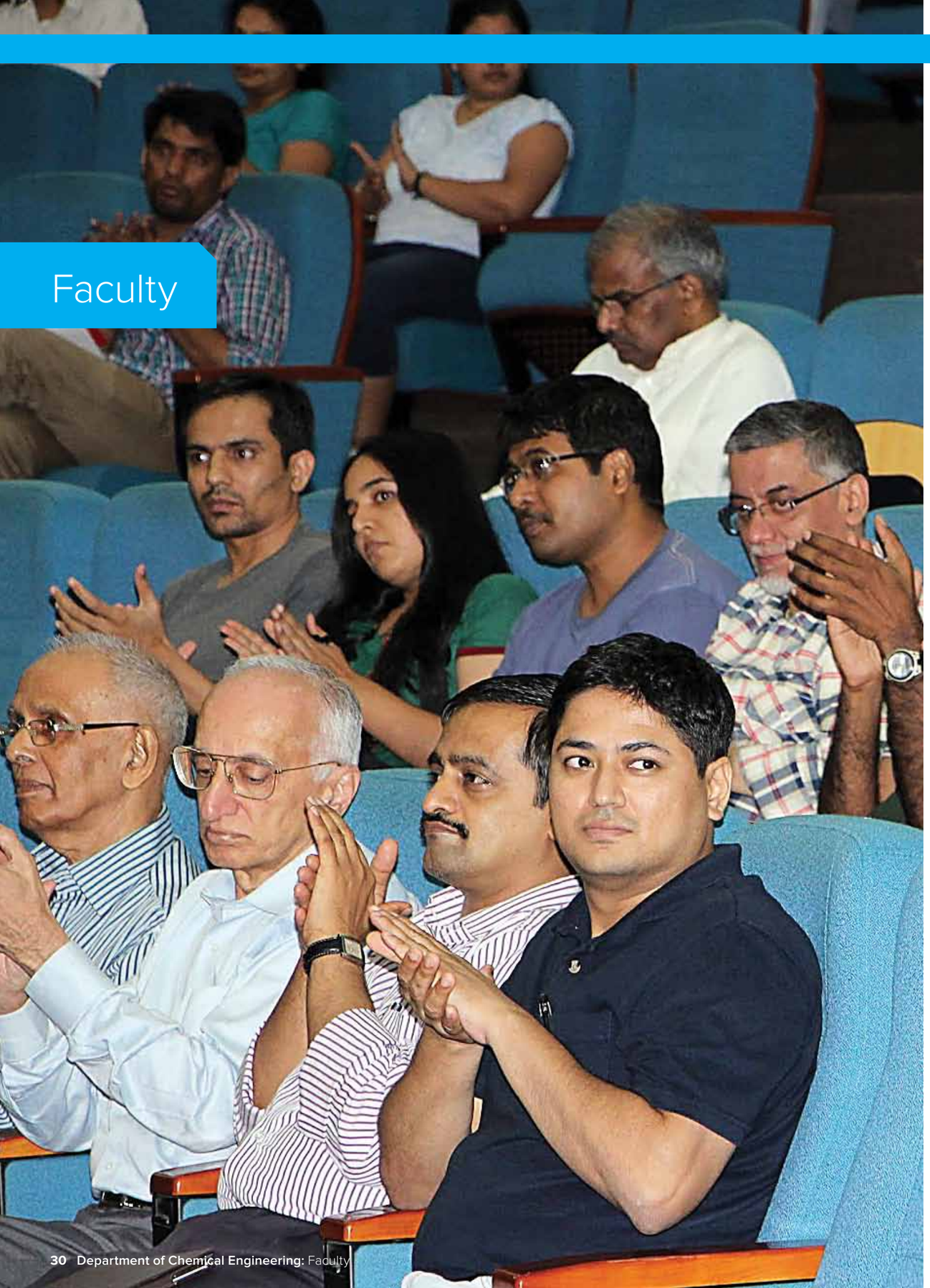
Catalysis and Reaction Engineering



The Reaction Engineering and Catalysis group pursues excellence in both theoretical and experimental aspects, targeting commercially important applications from a fundamental standpoint with a mix of classical and modern concepts and techniques. Thus, the focus of the group is on classical areas such as process design and optimization as well as modern areas such as biofuels (from raw materials to products), advanced energy technologies such as fuel cells, electro-synthesis of new products by green and sustainable technologies, catalysis (synthesis, characterization and performance evaluation) for fine chemicals, and chemical technologies for semiconductor applications (Chemical vapor deposition of silicon as an alternative to Czochralski process). Some of the research by the group is specific to India such as underground coal gasification of high ash content coals which is primarily available in India. In addition, the group is also engaged in providing smart engineering solutions to Indian Industries. The group has expertise both in theoretical aspects involving modeling and computational studies of industrial as well as bio-reactors and experimental aspects involving performance evaluation of scaled down reactors, electrochemical systems, catalyst synthesis and characterization etc. The emphasis of the group is always on fundamental understanding. The facilities available with the group and the department allow a multidimensional and multiscale understanding of the problems related to catalysis and reaction engineering. The students working on different aspects of catalysis and reaction engineering are trained on sophisticated instruments and advanced computational techniques which will be critical when they take positions in academia or industry. Thus the group serves a vital national interest in providing trained manpower. Quite often the spectrum of research on catalysis and reaction engineering intersect with chemistry, biology and materials science. Thus, the students are trained to learn and apply concepts and methodologies from these areas. The group encourages students to broaden the horizons of scientific learning and equips them with the tools to do so. As the group looks to the future, it aims to develop new chemicals and processes, green and viable technologies, process and technologies targeted to meet India's needs in terms of energy, environment and chemicals.

Process Systems Engineering

Process Systems Engineering (PSE) focuses on a complete, life cycle view of the manufacturing process in chemical engineering, beginning from the scale of molecule discovery & scale up to the other end of spectrum relating to achieving manufacturing excellence and minimizing environmental impact. The PSE research has been focusing on these various individual steps in the life cycle of process engineering from both theoretical as well application perspectives. Beginning at the smallest scale of molecular modeling, research work at the department has focused on Novel multi-scale simulation techniques for simulating complex interacting systems.The molecular scale information is employed with macroscopic models to describe chemical processes at the device length scales. Attempts to exploit the predictive capabilities of these multi-scale models for optimizing aforementioned devices are also currently underway. At the larger scale, the group has been focusing on the development of a generalized reactor model framework that can accommodate the wide diversity of chemical reactors. Establishing empirical cause and effect relationships for the purposes of process development, scale-up, process optimization, advanced process control, as well as fault detection and diagnosis, has been an area of significant activity in the systems engineering group. Basic and advanced optimization has been a focus area of research in the department with several important and critical applications. Optimization for sensor network design that balances different criteria, such as process observability, precision & accuracy of parameter estimates and fault isolability, and overall cost of the sensor network has been an another active research area of the group. The group also focuses on the design of energy efficient heat exchanger networks along with approaches to identify opportunities for process intensification, i.e evolving substantially smaller, cleaner, and more energy-efficient designs. Some of key applications that are being considered are design of novel reactive separations methods for important industrial systems and design of new and alternate process routes related to green manufacturing. Basic and advanced process control approaches are deployed in chemical process manufacturing to realize the optimal targets resulting from design and/or operational optimization steps. Model predictive control (MPC) has been one of the popular model based control algorithms. The group works on multi-parametric MPC approach with special applications to fast transient systems. Biological systems exhibit several interesting phenomena at the cell level such as significantly amplified sensitivity of enzyme cascades. To develop a better understanding of these interesting phenomena, control theoretic approaches have been successfully used to represent and explain the feedback-like structures at the cell level.



Faculty

Research Themes of Faculty

Faculty	Biosystems Engineering Research	Soft Matter Engineering	Process Systems Engineering	Reaction Engineering & Catalysis	Thermodynamics & Molecular Simulations	Energy Environment & Sustainability
CORE FACULTY						
Jhumpa Adhikari			★		★	
Rajdip Bandyopadhyaya		★				
Jayesh Bellare	★	★				
Sharad Bhartiya			★			
Mani Bhushan			★			
Abhijit Chatterjee			★	★	★	
Ratul Dasgupta		★				
Partha Sarathi Goswami		★				
Ravindra D Gudi			★			
Venkat Gundabala	★	★				
Sameer Jadhav	★					
Vinay A Juvekar		★		★		
Devang V Khakhar		★			★	
Sanjay M Mahajani			★	★		
Abhijit Majumder	★	★				
Ateeque Malani		★			★	
Ranjan K Malik			★			
Anurag Mehra		★		★		
Sarika Mehra	★					
Arun S Moharir			★			
Kannan M Moudgalya			★			
Hemant Nanavati						
Santosh Noronha	★					
Sachin C Patwardhan			★			
Sandip Roy		★				★
Supreet Saini	★					
Arindam Sarkar				★		
Jyoti Seth		★			★	
Yogendra Shastri			★			★
P Sunthar		★				
Akkihebbal K Suresh		★		★		
Rochish Madhukar Thaokar		★				
Mahesh S Tirumkudulu		★				
Mukta Tripathy		★			★	
Chandra Venkataraman		★				★
K V Venkatesh	★		★			
Madhu Vinjamur		★		★		
Ganesh A Viswanathan	★			★		
Pramod P Wangikar	★					★
PROFESSOR EMERITUS						
K P Madhavan			★			
A P Kudchadker			★		★	
VISITING FACULTY						
M S Ananth					★	
ADJUNCT FACULTY						
S Ganeshan			★			
Y S Mayya		★				★
Mamata Mukhopadhyay					★	
Vijay M Naik		★				★
Leja Hattiangadi			★			

Jhumpa Adhikari

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P: +91 (22) 2576 7245

Ph.D, University at Buffalo, 2004

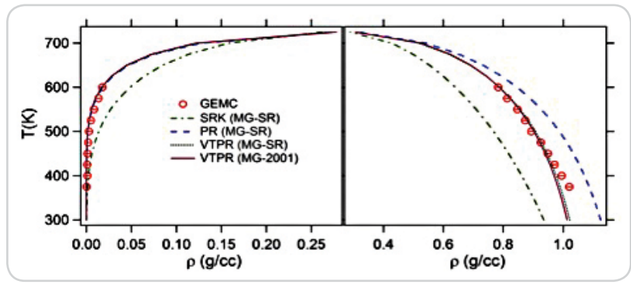
Jhumpa Adhikari

Areas of Interest: Thermodynamics, Statistical Mechanics, Molecular Simulations

Molecular Simulations techniques such as molecular dynamics and Monte Carlo simulations are used in the development of new methods for determination of free energies and phase equilibria of different systems. Our group has been working on the development of a multi-scale modelling scheme for compound semiconductors which find wide range of applications in the fabrication of opto-electronic devices. Other areas of research include performing molecular simulations to determine the adsorption behaviour and phase equilibria of confined fluids; and to study the impact of different factors such as strength of wall-fluid interactions, on these fluids. Further, the group is also employing the molecular simulation approach to generate phase equilibria data which are required in the design and optimization of polymerization process equipment. We are also working on the development of efficient molecular simulation techniques for phase equlibira predictions. The development of a generic computional scheme for rational solvent design is also in progress.

1. Computational schemes for rational solvent design

The group is also attempting to develop a computational scheme for rational solvent design to select the optimal solvent (or design a new solvent) for the extraction of a pharmaceutical intermediate synthesized using a biotransformation process. An additional step, whereby the cost-effective molecular simulation approach (the accuracy of this approach is limited only by that of the force field employed to model the interactions in the molecule) is used to verify the trends in the computer-aided molecular design results; has been introduced in the computational scheme. The molecular simulation techniques also allow us to gain molecular insights into the solvent extraction process.



VLE of Phenylacetylcarbinol

2. Prediction of thermodynamic properties for industrially important polymerization systems using molecular simulations

In this project, we will attempt to predict the VLE data for pure component monomers and their mixtures with different reactants/products at the operating conditions of the process equipment. This data, necessary for the design and optimization of process equipment, is generally not available or only very limited data is available in literature. We are presently focusing our research on the polyethylene polymerization system.

3. Design of compound semiconductor alloys using molecular simulations

Simulation of solids provide an unique challenge because of the high densities involved which preclude use of any of the well established insertion/deletion methods used in the fluid phases. This provides an opportunity for the development of new methods to successfully measure the free energy of the solids and to improve the efficiency of the techniques used. Molecular simulation techniques are applied to determine the solubility diagrams for solid solutions, such as ternary and quaternary compound semiconductor alloys, and also to predict the structural properties, local composition and thermophysical properties of the above mentioned alloys.

Publications:

1. M. Harini; Adhikari, Jhumpa and K. Yamuna Rani, **Prediction of vapour-liquid coexistence data of Phenylacetylcarbinol** Fluid Phase Equilibria (2014) 364, 6-14

2. Sengupta, Angan; Behera, Pratik and Jhumpa Adhikari, **Molecular simulation study of triangle-well fluids confined in slit pores** Molecular Physics(2014) 112 (15), 1969–1978

3. Rathi, Punit; Sikder, Sanjib and Jhumpa Adhikari, **Structural characterization of III-V zinc blende compound semiconductors using Monte Carlo simulations** Computational Materials Science (2012) 65, 122-126

Research in our group attempts to develop computational schemes to study and understand the behavior of solids and fluids; particularly phase behavior.

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Ph. D, Indian Institute of Science , 2000

Rajdip Bandyopadhyaya

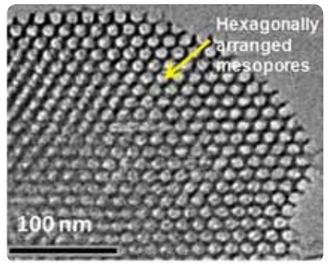
Areas of Interest: Nanoparticles, Water treatment, Drug Delivery, Modeling and Simulation

Our research draws on the principles of colloids and interfacial science to study synthesis, properties and applications of nanoparticles. The emphasis is on understanding the dynamics between various reactant and template molecules and the resultant nanoparticulate product (either a dry solid or a dispersion) in a complex, multiphase system. This is achieved by explaining interaction across multiple time and length scales that govern phenomena in both microscopic (reactant) and mesoscopic (nanoparticle-level) scales. Both experimental and modeling tools are used in conjunction, so as to develop further insight into relevant applications.

Along these lines, the first track in our research is to develop from molecular principles, a suite of porous hosts (mesoporous silica, porous carbon etc.), with different geometry and dimension of particles and internal pores. This can aid breakthrough in designing nanomaterial hybrids for catalysis, water disinfection and drug delivery. Further in this regard, a unified model of such a porous host with an impregnated second nano-dimensional additive is being developed, (combining diffusion, adsorption and reaction), in order to explain experimental trends and optimize performance of these hybrids. A second track is to develop a general mathematical model for addressing both size and shape-controlled, solid (iron oxide, silver, cerium oxide, titanium oxide) nanoparticle synthesis, to predict features both at individual nanoparticle-level and at the larger aggregate-level of several primary particles. This can be coupled to the conservation equations of transport and chemical kinetics, so that nanoparticles can be made in large quantities in a scaled-up reactor.

1. Porous hybrid nanomaterials for catalysis and drug delivery

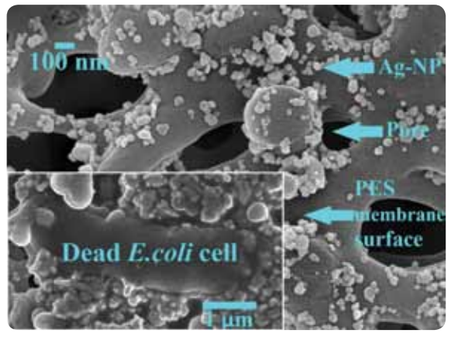
We have made various porous nanomaterials, with precise geometrical features and chemical functionalities, each having a unimodal pore diameter in the range of 2.5-12 nm. These are a high surface area host, within which a second nanoparticle, drug or enzyme has been impregnated to generate hybrid materials with high reactivity. For example, TiO_2 nanoparticle loaded SBA-15 has been developed to photocatalytically degrade water-soluble dyes at a very high rate. In contrast, drug loaded SBA-15 has been shown to kill cancer-cells in a pH and receptor-specific targeted manner.



TEM image showing well ordered nanometer-sized pores in a mesoporous silica particle.

2. Silver nanoparticle incorporated packed beds and membranes for water disinfection

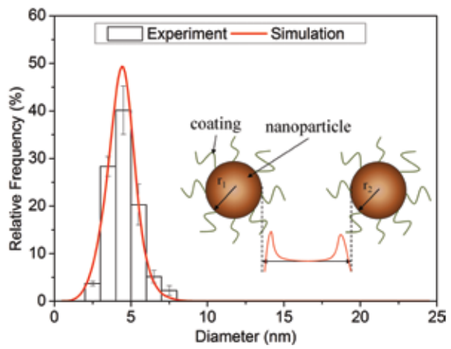
Household drinking water purification systems using activated carbon (AC) as the filtration medium suffer from biofouling, which can be eliminated by using the biocidal effect of silver (Ag). Employing an innovative plasma- treatment method, we have achieved superior impregnation of Ag nanoparticle (Ag-NP) in AC (Ag-AC). This hybrid achieved complete water-disinfection in a continuous column-operation, combining high kill-rate of E. coli coupled with a low rate of Ag release. Extending further, a lab-scale cross-flow membrane module has been designed to demonstrate anti-biofouling activity of Ag-NP impregnated sulphonated polyethersulfone (SPES) membrane. Currently, we are pursuing impregnation of other nanoparticles in AC, to achieve removal of other contaminants from water.



Silver nanoparticle incorporated polyethersulfone (Ag-SPES) membrane shows (inset) a dead E.coli cell in biofouling prevention.

3. Modeling and simulation of complete nanoparticle size-distribution

A major challenge in nanoparticle research is to specify experimental conditions for manufacturing nearly-monodisperse nanoparticle samples. We have shown that by using a model consisting of nucleation, diffusion-growth and coagulation-growth, one can a-priori predict, without any fitting parameter, the complete particle size distribution (PSD) of both uncoated and coated primary nanoparticles. This has been possible by using an interparticle potential function based Monte Carlo simulation, which accurately captures the physics of coagulation. This can be a general framework to predict PSD of all types of nanostructures of any material.



Dextran coated Fe_3O_4 nanoparticle size distribution, based on interparticle interaction shown schematically.

Publications:

1. Kumar, S., Ravikumar, C., Bandyopadhyaya, R., State of Dispersion of Magnetic Nanoparticles in an Aqueous Medium: Experiments and Monte Carlo Simulation, **Langmuir,** 2010, 26(23), 18320-18330.

2. Srinivasan, N. R., Shankar, P. A., Bandyopadhyaya, R., Plasma treated activated carbon impregnated with silver nanoparticles for improved antibacterial effect in water disinfection, **Carbon,** 2013, 57, 1-10.

3. Padwal, P., Bandyopadhyaya, R., Mehra, S, Polyacrylic acid-coated iron oxide nanoparticles for targeting drug resistance in mycobacteria, **Langmuir,** 2014, 30(50), 15266-15276.

We focus on synthesizing nanoparticles and functionalizing them, for both improving existing and developing new applications, thereby harnessing their intrinsic advantages into engineered solutions.

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Ph.D, U. Minnesota, Minneapolis, 1988

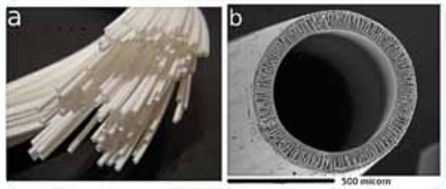
Jayesh Bellare

Areas of Interest: Nanotechnology, Electron Microscopy, Healthcare, Medical devices.
Plus: Soft nanomatter, Hollow fibre Membranes; Bone tissue engineering; Nanomedicines; Ayurvedic and Homeopathic medicines; Scaffold Development for Stem Cell Expansion; Patent Ductus Arteriosus Occlusion Device.

My group focuses on the cross-disciplinary area of nanotechnology for human healthcare. This involves nanostructured materials, nanomedicines, biomedical devices and cryo-electron microscopy, using soft and safe materials. Our studies are fundamental as well as applied. We collaborate extensively, internally with many IIT colleagues, and externally with several leading institutions, labs and doctors. Our work is proven not only through papers and patents but also through their applications reaching industry and medicinal use, or getting very close to it. Currently we are seized with the regulatory processes of getting products approved for human trials. Our work includes nanoparticles for drug delivery, biomedical devices, tissue-engineered bone grafts, nanoclay-polymers, hollow-fiber dialysis membranes, complex liquids, soft solids and stem cells, particularly their expansion with 3D scaffolds. Of particular significance is our pioneering work on nano-medicines that spans all three medicinal systems: Allopathic (“modern”), Ayurvedic (“traditional”) and Homeopathic (“alternative”). Our nano-carboplatin is the first Indian nanomedicine to reach human trials for retinoblastoma. We showed the nanoparticle basis of super-dilute Homeopathic medicines, explaining a century-old controversy relating to super-Avogadro dilution. Holes in hearts and other defects in newborn babies can be resolved better with our new design of occlusion devices for minimally invasive surgery. Our hollow fiber membranes with nano-additives would impact kidney dialysis significantly. Our work in nano-bioengineering hopes to have an enduring influence on healthcare technologies.

1. Hollow fiber membrane for biomedical application

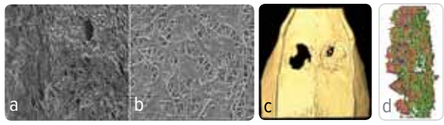
End stage renal disease (ESRD) is the complete failure of kidney functions, where kidneys can no longer remove wastes, concentrate urine, and regulate many other important body functions. Hemodialysis is one the most effective and widely used mode to regulate the kidney functions artificially. The hemodialyzer cartridge (disposable blood filter) is the key component of this treatment technology and is currently imported. At the Department of Chemical Engineering, we have successfully developed an indigenous and low-cost technology for continuous pilot-scale production of hollow fiber membranes to be used in hemodialysis and built prototype microdialyser. Our formulated special antioxidative composite polsulfone/vit E TPGS membrane material improves the performance in both separation and biocompatibility front. This will permit faster treatment, lesser side reactions and could spur novel devices like portable/wearable dialysers. Along with these we have also used the HFM technology in making a step towards bioartificial organs like bioartificial liver and bioartificial pancreas.



Picture of the prepared HFM bundles and b) SEM micrograph of the HFM showing asymmetric structure, porosity and uniform structure.

2. Nano-biocomposite Bone Grafts for Reconstructive Surgery

Bone grafts are frequently used in surgical interventions for such skeletal deficiencies and are second to blood transfusion on the list of transplanted materials. We have developed ideal bone graft by preparing electrospun membranous 2D nano-fibers and biodegradable 3D composites as a biomimetic scaffold. The scaffolds have shown promising performance both in-vitro and in-vivo. Thus, the new materials developed here are ready for human clinical trials and could help in fast healing of various dentistry and orthopaedics.



SEM micrographs to demonstrate morphology and microstructure of composite (a) MG63 culture cell on 3D Scaffold; (b) MG63 culture cell on membranous Scaffold; (c) Reconstructed 3D micro-CT images of rat calvaria implanted with PGH scaffold 10 weeks (10 W) at single side (right) and the other side was blank; (d) Restored 3D model of the newly formed bone using combined effects of CTan and Mimics of entire defects treated with nHA-CMChNa-GEL scaffold composites operated defects at week 07 respectively (the threshold employed were 1-147 Hounsfield units (HU) for soft tissue, 148-661 HU for adult spongial bone and 662-1988 HU for adult compact bone as represented by green, red and blue color respectively)

3. Scaffold Development for Stem Cell Expansion

Stem cell therapy and tissue engineering have emerged rapidly due to the limitations associated with organ transplants such as immune rejection and donor site morbidity. Stem cells are special kind of cells which have ability to renew itself and as well as to differentiate into different kinds of cells. The problem with cell therapy is that low number of cells is obtained from single donor that is not sufficient for transplantation and when they are cultured in vitro, the cells lose their renewal capacity and start to differentiate. To address these issues, our research is focused on development of scaffold that allows proliferation of stem cell as well as maintains their pluripotency. We study how scaffold properties can be modulated to assess the role of cues in affecting stem cell fate and how this system can be used to improve stem cell-based therapies.

Publications

1. Dahe GJ, Teotia RS, Kadam SS, Bellare JR (2011). The biocompatibility and separation performance of antioxidative polysulfone/vitamin E TPGS composite hollow fiber membranes. Biomaterials 32:352-365.

2. Sagar N, Pandey AK, Gurbani D, Khan K, Singh D, Chaudhari BP, Soni VP, Chattopadhyay N, Dhawan A, Bellare, JR (2013). In-Vivo Efficacy of Compliant 3D Nano-Composite in Critical-Size Bone Defect Repair: A Six Month Preclinical Study in Rabbit. PLOS ONE 8: e77578.

“Prof. Jayesh Bellare is a recognized world leader the cross-disciplinary, emerging area of nanotechnology, microengineering and ultra-microscopy. The significance of his work has been to understand chemical engineering and bioengineering at a microscopic and nanoscopic level using the tools of cryo-electron microscopy, and scale the results to industrially relevant systems.”
(from the National Academy of Sciences, India, fellowship citation)

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Sharad Bhartiya

Areas of Interest: Optimal operation of simulated moving beds; Operation and control of fuel cells; Economic potential of algal bio-fuels; modelling, estimation and control of hybrid dynamic systems; systems biology of yeast

Our research focuses at the intersection of dynamic modelling, estimation, control and optimization of industrially relevant systems as well as naturally occurring systems. We use first-principles models to obtain optimal methods of operation. Feedback is incorporated with online plant data to devise advanced control strategies such as Model Predictive Control. Our work also involves developing novel algorithms as well as mathematical formulations for fast control. In the applications domain, we are currently focussing on novel ways of operating simulated moving beds, developing refinery-wide techno-economic models for algal biorefinery, as well as control and operation of a solar thermal power plant. In the systems biology area, our work involves deciphering the principles of regulation recruited by naturally occurring systems. We primarily focus on yeast systems and have studied the integral control architecture in osmoadaptation response, role of multiple phosphatases in cell cycle regulation, and evolution of galactose uptake regulation. Our approach mainly consists of taking a system/ control theoretic approach to studying these problems.

1. Simulated Moving Bed Chromatography (SMBC):

Optimal operation of SMBC involves determining the internal flow rates and switch time that yield a cyclic steady state corresponding to an optimal performance metric such as feed throughput or productivity. Our work envisages using dynamic optimization using SMBC models to determining these best operations. The work also covers optimal start-up, recovering from feed upsets, transitions between optimal operating modes, and flexible ways of operation such as multi-period operation. An in-house fabricated SMBC for separation of a glucose-fructose system and capable of computer controlled operation is being tested.

Experimental SMBC Setup

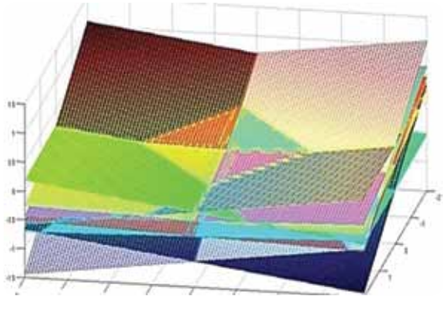
2. Explicit Model Predictive Control (e-MPC) of fuel cell and gas turbine systems:

MPC of fast dynamic systems has always been a challenging task, the main hurdle being the time required to calculate the constrained optimization problem at each sample. e-MPC has emerged as one way of arranging these computations. However, a number of issues need to be overcome before this technology can mature. Our work is progressing on two fronts: use of multiple models in e-MPC and developing new ways of solving the point-location problem (solved online in e-MPC). The multiple model approach envisages nonlinear compensation via use of multiple linear models with some form of convex aggregation. Optimzation based on multi-parametric programming leads to an offline generation of numerous regions which must be searched online to determine the location of the current operating point. We are collaborating with Prof. Mani Bhushan to explore discriminant function approaches for this point location problem. The applications include fuel cell and gas turbine systems.

Benchmark 3-Tank System

3. Control of Hybrid Dynamic Systems (HDS):

Hybrid dynamic systems involve interactions between continuous (such as in transport models) and discrete variables (such as in switching of dynamics). Constrained optimal control or MPC of such systems require solutions of MIQP/LP/NLP. Our work attempts to reformulate the control problems using set-theoretic methods ease online computing while guaranteeing stability. In particular, we proposed a dual terminal set approach that allows an efficient solution of the online optimization problem in MPC. The work is being extended to robust control using tube-based formulations as well as robust adaptive extensions using range inclusion functions.



Critical Regions in Explicit MPC

Publications:

1. A. Gupta, S. Bhartiya*, P.S.V. Nataraj, “A novel approach to multiparametric quadratic programming”, Automatica 47, 2112-2117, (2011)

2. K. Hariprasad, S. Bhartiya, R.D. Gudi, “A gap metric based multiple model approach for nonlinear switched systems”, Journal of Process Control 22 (9) , 1743-1754, (2012)

3. K.K. Kottakki, S. Bhartiya , M. Bhushan, “State estimation of nonlinear dynamical systems using nonlinear update based Unscented Gaussian Sum Filter”, Journal of Process Control, 24(9), 1425-1443, (2014)

Our major work lies in developing reformulations for dynamic optimization, model predictive control and state estimation with a view towards efficient solutions, nonlinear compensation and robust stability. Our applications include engineered as well as natural systems.

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Mani Bhushan

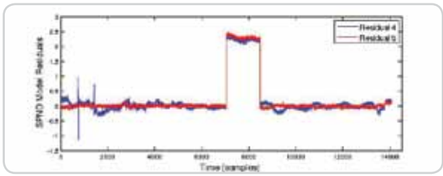
Areas of Interest: Sensor network design and audit; nonlinear, constrained state estimation; data analysis

The main focus of our research is in development of tools and techniques that aid in optimal and safe process operation. To achieve this, an essential step is to first ensure that the key variables are being measured in the process. We thus focus on development of approaches that can help in selecting an optimal set of measurements to ensure optimization of various objectives, such as those related to fault isolation and state estimation. At the operational level, we work in development of efficient but accurate state estimation techniques for nonlinear systems. These techniques use predictions from an uncertain process model in combination with noisy and incomplete process measurements to estimate important process states and parameters of interest. In particular, our focus has been on deterministic sampling and optimization based approaches that can estimate states in presence of constraints on states.

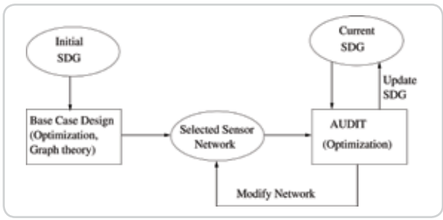
On the applications side, we apply various data analysis tools to problems arising in energy and environment domain. In particular, we are working on using data driven techniques to quantify published mechanisms as well as identify newer mechanisms that characterize impact of aerosols on precipitation over the Indian subcontinent. We are also using data driven techniques, namely principal component analyses and its derivatives, to develop a computationally efficient framework for detecting faults in flux measuring sensors in a nuclear power reactor in real-time.

1. Base case design and audit of sensor networks:

With thousands of variables in a typical chemical process, choosing the appropriate set of variables to measure is a non-trivial task. We have been working on developing graph based and constrained optimization approaches that can enable design of a sensor network, i.e. decide what variables to measure in a process, to ensure efficient fault detection and isolation. Apart from base case design methodologies, we have also developed approaches that can audit an existing sensor network. Non-informative sensors can also be identified whose removal does not affect the performance of the sensor network for a specified task. Such information can help in designing appropriate operator interfaces for different scenarios. Our work is based on signed digraph models that can be easily generated, even at the design stage, without requiring detailed process information. Currently, we are investigating design of sensor networks that can isolate various faults along with simultaneously identifying changes in the underlying digraph representation.



PCA Residuals



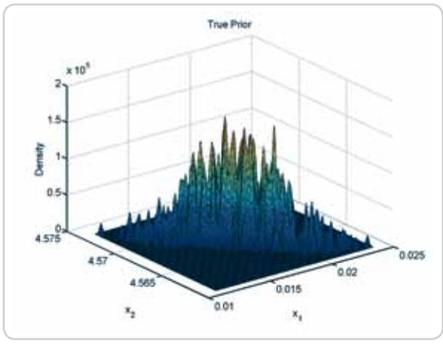
Sensor Network Design: Framework

2. Deterministic sampling based nonlinear, constrained state estimation:

To ensure efficient process operations, we are working on development of computationally efficient but accurate state estimation techniques for nonlinear systems. In particular, we have developed efficient, optimization based deterministic sampling based approaches that lead to estimates of states that satisfy the known constraints on the states. Initially focussed on variations of unscented Kalman filter that intrinsically assumes Gaussianity assumption, of late, we have been extending these ideas to a Gaussian sum unscented Kalman filter, that does not invoke Gaussianity assumption.

3. Data driven approaches for real time monitoring of self powered neutron detectors (SPNDs):

A typical nuclear power reactor can have hundreds of SPNDs spread throughout the reactor core, measuring the neutron flux distribution in the reactor. These detectors fail over a period of time but cannot be easily replaced as that entails reactor shutdown. In collaboration with BARC and NPCIL, we have developed data driven approaches that can (a) detect if a detector is faulty, and (b) provide an estimate of the true flux value corresponding to the faulty detector. In particular, we have used clustering and principal component analysis (PCA) based approaches to develop multiple linear models that enable fault detection, isolation and reconstruction. Currently, implementation in a real-time environment is being pursued to further test the applicability and performance of the proposed approach.



State Density

Appropriate selection of variables to be measured is not just a one time activity. It has to be supplemented with audit at regular intervals to identify opportunities for improving the performance of the network. Approaches based on signed digraph representation can provide useful information in this analysis.

Publications:

1. S. Kolluri, M. Bhushan, 2013, Audit of Sensor Networks for Efficient Fault Diagnosis, Journal of Process Control, 23, 881-893.

2. S. C. Kadu, M. Bhushan, K. Roy, 2013, Optimization-Based Sigma Points Selection for Constrained State Estimation, Industrial & Engineering Chemistry Research, 52, 1916-1926.

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Ph.D, University of Delaware, 2007

Abhijit Chatterjee

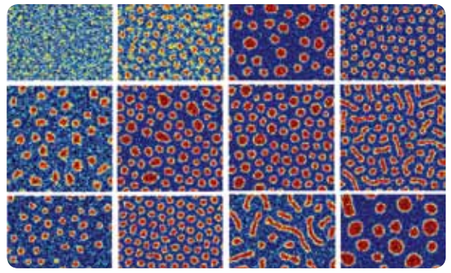
Areas of Interest: Reaction engg and catalysis, Thermodynamics and molecular simulations, Energy

Rapid development of alternative, efficient energy technologies is needed to tackle the impending crisis resulting from energy security, climate change and depleting natural resources. My research group is working towards building computer simulation tools that can contribute to such efforts. We study using a variety of simulation techniques developed in our group the mechanisms associated with reaction and diffusion processes in materials used in novel energy devices. These first principles simulations-based insights could be used in the future to guide selection of alternative materials for these energy applications. Although computational modeling and simulation has traditionally played an important role in chemical process design, controlling reaction and transport processes spanning multiple length and time scale in these new technologies introduces unprecedented challenges. Motivated by the scientific and technological challenges that plague novel device design, our main goal consists of developing systematic computer-aided rational materials design strategies using state-of-the-art multiscale modeling methods. Some of applications we are studying using our multiscale models include batteries, fuel cells, opto-electronic devices, nuclear reactor materials, and heterogeneous catalysis.

We achieve a multiscale view of materials by combining traditional molecular-level simulation techniques such as density functional theory, molecular dynamics and Monte Carlo with recent advances from our group in methods like the Accelerated Molecular Dynamics techniques (AMD), Kinetic Monte Carlo (KMC) and Continuum mesoscopic equations (CME).

1. Development of multiscale simulation techniques

Our goal is to gain a fundamental understanding of the interplay between ionic transport and material structure in the battery and fuel cell electrode and electrolyte materials. Unfortunately, computational methods which can provide this understanding are lacking because transport in these devices span multiple length and time scales, ranging from atomic scales to centimeters, and from picosecond to hour time scales. While continuum are computationally inexpensive, they do not predict the transport properties accurately. On the other hand, atomistic methods are computationally very expensive for studying this multiscale phenomena. State-of-the-art multiscale modeling techniques developed in our research group overcome these challenges and will be employed to study ionic transports in energy storage and conversion materials.



Self-assembled structures obtained in heteroepitaxial system as the growth conditions are varied. The structures are predicted using our computational framework.

2. Material informatics for energy applications

Our approach for extracting the connection between the materials used in the device and the device performance can be termed as a materials informatics approach. The main idea involves building large databases that describe the underlying materials physics and chemistry spanning multiple length and time scales using accurate computer models, and process this data using informatics tools to achieve insights into materials behavior which could later be used for rationally design materials for energy applications. Detailed kinetic models can provide us with the understanding of how the material used in the device influences the kinetic behaviour from molecular to device length scales.

Publications:

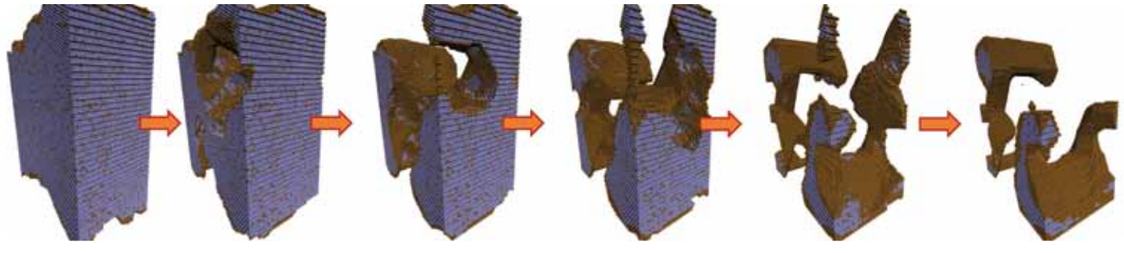
1. Paramita Haldar and A. Chatterjee, Many-atom surface processes are relevant to the structural evolution of metal nanoparticles, Modelling Simul. Mater. Sci. Eng. 23, 025002, 2015.

2. Srikanth Divi and A. Chatterjee, Accelerating rare events while overcoming the low-barrier problem using a temperature program, The Journal of Chemical Physics 140 (18), 184116, 2014

3. Rehman T., M. Jaipal, and A. Chatterjee, A cluster expansion model for predicting activation barrier of atomic processes, J. Computational Physics, 2013, 243, 244-259.

The computational methods we have developed recently could play an important role in our ongoing search for alternate materials for a broad range of energy applications.

Example of materials structure evolution observed during a typical chemical dissolution processes used for synthesis of materials for energy applications.



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Ph. D, Jawaharlal Nehru Centre for Advanced Scientific Research, 2010

Ratul Dasgupta

Areas of Interest: Interfacial flows, Waves in fluids and their stability, Mechanical response of amorphous materials.

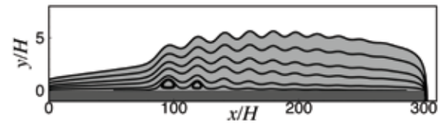
Our group studies problems in fluid and solid mechanics using analytical tools (like perturbative techniques) and computational tools (like Direct Numerical Simulations for fluids or Atomistic simulations for solids). We take up problems of a basic or applied nature and try to understand the associated physics. What we work on, can be broadly organised into two headings -

• **Interfacial flows, waves and their stability** - From the complex interference patterns generated by rain-drops falling on a pool to the myriad surface patterns of an open ocean: the complexities of a deformed fluid interface is an abundant source of puzzling fluid mechanical problems. Will a droplet falling on a pool lead to a splash? At larger scales, the coupling between the ocean and the atmosphere (air-sea interactions) is significant for weather-forecasting. The transport of sediments by waves is of interest in environmental problems of erosion etc. We study falling droplets, wave patterns in laminar air-water interfaces and hydraulic jumps analytically and computationally. We also plan to build a small laboratory to do some related experiments.

• **Mechanical response of amorphous materials** A large class of materials share a common attribute viz. an underlying disordered structure. The rheological response of these materials is interesting and not very well understood from first principles. When subject to mechanical deformation, their plastic response remains intertwined with elastic behaviour and developing an analytical framework is challenging. We propose to build on our recent work in this area towards a better understanding of plasticity in soft amorphous solids.

1. Droplet and jet dynamics

The man-made and natural world around us abounds in jets and water droplets. Their interactions with each other and with the surfaces with which they collide, can produce a very wide range of outcomes some of which can be visually very captivating. We seek a deeper understanding of how are droplets generated, dynamics of mutual impact of droplets and coalescence, the different modes of spreading on rigid and flexible surfaces, the dynamics of jet impact on rigid surfaces and the various hydrodynamic instabilities which arise as a part of these processes. This understanding is technologically very relevant - many manufacturing processes deal with droplets and jet impact and associated heat transfer. An improved understanding leads to an improvement in the efficiency and design of such processes. We are currently developing the necessary computational and experimental tools for studying this broad class of problems.



An undular viscous hydraulic jump

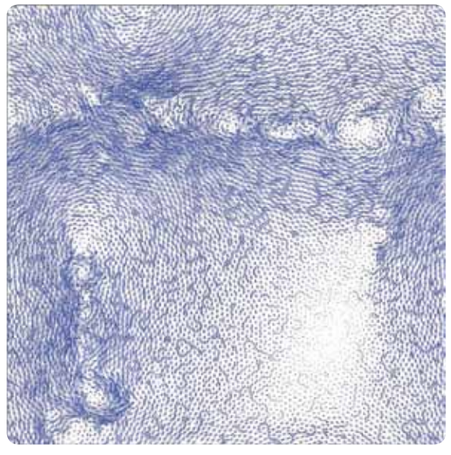
2. Waves on interfaces

We have a long-term interest in waves on interfaces, their stability and associated mass transport. One of the first problems under experimental study is wave formation on a flow down an inclined plane. This effort will soon be extended to computations and theory.

Wave pattern on a flowing stream

3. Plasticity in amorphous solids

In collaboration with colleagues at TIFR Centre for Interdisciplinary Sciences, Hyderabad (TCIS), we are conducting atomistic simulations of amorphous materials which sheds light into their plastic deformation. This is part of our ongoing work on understanding plasticity, shear-banding and fracture in amorphous solids.



Shear bands in atomistic simulations of amorphous solids

Publications:

1. Numerical simulation of laminar, standing hydraulic jumps in a planar geometry, Ratul Dasgupta, Gaurav Tomar and Rama Govindarajan, European Phys. Journal E (2015) (Accepted, To Appear).

2. The effect of initial momentum-flux on the circular hydraulic jump, Vishwanath K. P, Ratul Dasgupta, Rama Govindarajan and K. R. Sreenivas, ASME J. Fluids Engg., 137(6), 061301 (2015)

3. Microscopic Mechanism of Shear Bands in Amorphous Solids, Ratul Dasgupta, H. George E. Hentschel, and Itamar Procaccia, Phys. Rev. Lett. 109, 255502, (2012).

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Partha S Goswami

Areas of Interest: Turbulent suspensions, inertial migration, particle image velocimetry (PIV)

Our research focuses on the exploring the dynamical behavior of fluid-particle suspensions for a wide range of flows like micro flow to large-scale particle laden turbulent flows. We are mainly interested in exploring the interactions of fluid and particles in suspensions. We combine advanced experimental technique like particle image velocimetry (PIV) and numerical simulations (DNS) to understand the physics of such interactions. We also put our efforts to model such flows using statistical mechanics at least in some limiting cases. In case of turbulent particle laden flows, there are strong coupling between the turbulent fluctuations in the fluid velocity fields, and the fluctuating velocities of the particles. Owing to this simultaneous analysis of both the phases give insight to model large scale engineering systems. Another area of our interest is inertial microfluidics. In general microfluidic devices operates at very low flow rates. Because of very low dimension of the channel and low flow rate fluid phase Reynolds number in general is very low. Due to this it is a common idea that in case of microfluidics, inertia does not play any significant role. But there are few novel applications where inertia plays important role. Two major examples are secondary flow generation in a microchannel and inertial migration of the particles. We aim to investigate the combined effect of secondary flow and inertial particle migration on particle focusing using numerical simulations and experiments.

1. Dynamics of particle laden turbulent flows: experiments and modeling:

Particle-laden turbulent flows find applications in many industrial processes like pneumatic transport of powders, coal combustion, fluidized bed reactors etc. Turbulence plays important role in both the distribution and de-mixing/segregation of the particles. Depending on the intensity of the turbulence and particle inertia, higher particle concentration may happen near the wall region of the flow geometry which may cause higher rate of particle deposition at the wall. A proper understanding will lead to the assessment of deposition behavior and the transport coefficients in the above mentioned processes. In the proposed project we plan to conduct experiments and simulations to predict dynamics of both the phases simultaneously. Simulation will be performed based on fluid-particle coupled model (two way coupling) such as large eddy simulation (LES) for fluid phase with discrete element model (DEM) for particle phase. Experiments using particle image velocimetry (PIV) will be conducted and compared with simulation results.

2. Dynamics of inertial suspension in microchannel:

The proposed research deals with the theoretical and experimental investigation of the dynamics of inertial suspension in microchannel. Even though the flow Reynolds number is low, during its motion in confined channel the constituent particle of suspension experiences inertial lift force, which in turn produces particle migration. Such migration behavior of the particle can be utilized to develop filter-less separation technology based on particle shape and size. Here we plan to apply fully resolved lattice Boltzmann method (LBM) to numerically simulate the dynamics of particle and fluid flow behavior for spherical and non-spherical. Experiments will be conducted using in-house-developed micro-PIV technique to validate the theoretical results.

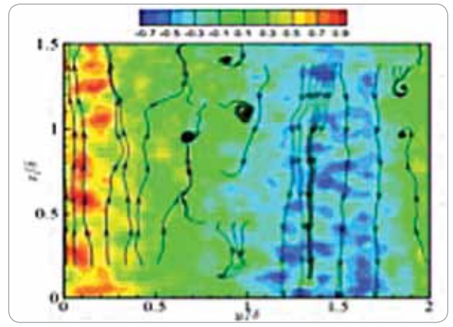
3. Modeling and experiments on chemical vapor deposition process in fluidized and spouted bed:

The fluidized/spouted bed technology is widely applied in pharmaceutical, chemical and petrochemical industries. Such technology can be applied for coating, surface modification of the particles using chemical vapor deposition (CVD). To control the deposition process a detail understanding of simultaneous hydrodynamics of gas-solid phases, reaction kinetics, and mass transport processes are required. Therefore it is required to develop a composite model to address hydrodynamics and local kinetics to address the overall coating process on the particle.

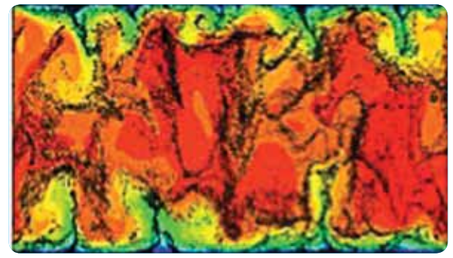
Publications:

1. P. S. Goswami, V. Kumaran, Particle dynamics in a turbulent particle-gas suspension at high Stokes number. Part 2: The fluctuating force model. Journal of Fluid Mechanics, 646, 91–125 (2010).

2. P. S. Goswami, V. Kumaran, Particle dynamics in the channel flow of a turbulent particle-gas suspension at high Stokes number. Part 1: DNS and fluctuating force model. Journal of Fluid Mechanics, 687, 1–40 (2011).



Particle induced turbulence: Experiments



Particle clustering in turbulent flows: DNS

PIV facility

Study on inertial microfluidics leads to develop filter-less separation technology.

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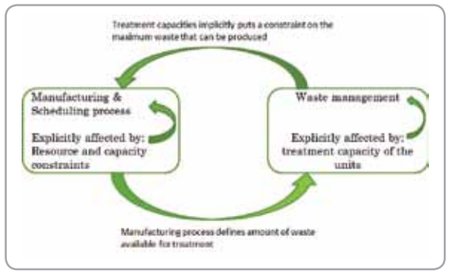
Ravindra D Gudi

Areas of Interest: Process Systems Engineering, Process Performance and Energy Audit, Optimization & Control, Green Engineering

Process systems engineering focuses on a holistic view of the system to understand the cause-and-effect relationships and interactions between different sub-systems, that impact the overall system performance. This understanding can be exploited to develop optimal decisions for efficient and green designs of process plants, as well as to operate these plants safely, profitably and with minimal environmental impact. The PSE approaches of modeling, optimization and control along with statistical methods also help to develop optimal, fault-tolerant operating methodologies. These approaches further help in performance analysis to establish benchmarks for plant performance, grade the current plant performance against these benchmarks and diagnose / remedy factors that are responsible for sub-optimal performance. Work in my research group has predominantly been in the PSE area with applications in energy generation, pharmaceutical and health sciences related manufacturing, and process manufacturing in both continuous and batch modes.

1. Decomposition based approaches for optimization and control:

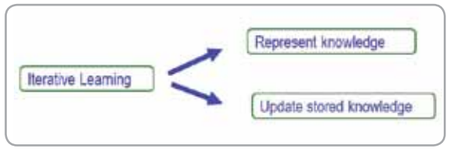
Large scale optimization problems, resulting from analysis of enterprise wide optimization & control objectives, are usually daunted by complexity related to size. Model based and goal based decomposition and co-ordination methods help to simplify the complexity by decomposing the larger, central problem into smaller sub-problems that have a greater possibility of being solved to local optimality. A co-ordination/ co-operation between these sub-systems then helps towards recovering the global optimality of the overall system. Such approaches also offer merits towards permitting additional degrees of freedom for solving the local optimization problems. Work in my research group has focused on analyzing approaches to reduce complexity in optimization problems posed in the areas of scheduling and decision support as well as large scale enterprise wide optimization (such as oil & gas production).



Integration of Manufacturing and Waste Management

2. Learning theory based approaches for PSE:

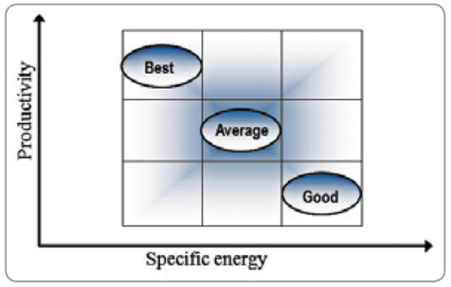
The main tenet of good manufacturing practice (GMP) requires that robust process designs are complemented by continuous improvement based manufacturing strategies. In a typical product development and manufacturing lifecycle beginning from bench scale to full scale, a lot of useful data is generated and archived. The wealth of information present in this data could be exploited towards generating an improved understanding of the cause-effect relationships. This improved understanding could be translated in terms of developing more accurate models that would help in generating realistic and optimal operating policies. Work in my research group has focused on exploiting advances in learning theory to develop improved dynamic models and hence better operating strategies/ recipes for batch and continuous process manufacturing.



Iterative learning and Operations Excellence

3. Integration issues in Renewable Energy Generation:

Feedstock for renewable fuels is usually sourced from a diversity of sources, that results in significant variation in its quality. The scalability of these renewable energy generation technologies is therefore reliant on a tight integration of energy generation with feedstock diversity. Aspects related to selectivity and severity of feedstock assimilation and the overall dynamics of the conversion process impacts the overall response times of the energy generation unit to varying/ fluctuating demand patterns. Research work in my group is currently focused on analyzing these integration issues both in the context of energy generation as well as waste valorization.



Performance classification and Targeting

Publications:

1. PR Kotecha, M Bhushan, RD Gudi, Efficient optimization strategies with constraint programming, AIChE journal 56 (2), 387-404, (2010).

2. RN Methekar, SC Patwardhan, R Rengaswamy, RD Gudi, V Prasad, Control of proton exchange membrane fuel cells using data driven state space models, Chemical Engineering Research and Design 88 (7), 861-874, (2010).

3. AS Badwe, RD Gudi, RS Patwardhan, SL Shah, SC Patwardhan Detection of model-plant mismatch in MPC applications Journal of Process Control 19 (8), 1305-1313, (2009).

Research work in my group has been in the broad area of process systems engineering, viz. modeling, optimization, control, and fault diagnosis with applications in the areas of energy generation, waste valorization, batch and continuous process manufacturing.

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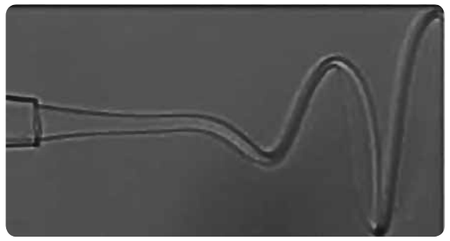
Venkat Gundabala

Areas of Interest: Microfluidics, Water-based coatings, Electrohydrodynamics, Micro and Nano particles

The thrust area of research in our group is Microfluidics. We use microfluidics as a platform for material synthesis and biological studies. In the area of material synthesis, we design and develop microfluidic devices to synthesize micro-particles, micro and naofibers, etc. for cell encapsulation and other applications. We also develop microfluidic platforms for biological applications like cell sorting, blood fractionation, etc. Our other area of prime interest is water-based coatings. We synthesize and investigate properties of nanocomposite water-based coatings with antimicrobial properties.

1. Microfluidics based approach to microencapsulation of multiple cells:

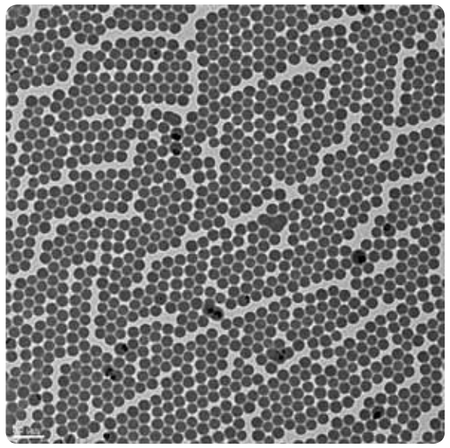
Cell microencapsulation is one of the most elegant and emerging approaches to targeted cell-based drug delivery. The technique involves immobilization of drug–laden cells inside a semi-permeable membrane, usually a polymeric microparticle. This approach overcomes the graft rejection problem usually associated with cell transplantation. Microfluidics offers a promising route to generation of polymeric microparticles which act as carriers of the drug-laden cells. The low flow rates involved in microfluidics allow precise control on the size of the microparticles. In this project, we are developing a microfluidics based technique for the controlled generation of polymeric microparticles and the subsequent encapsulation of drug laden cells. The idea is to develop a core-shell morphology which will allow encapsulation of multiple types of cells within the same particle providing distinct advantage over single cell type carrying particles. The project involves cell viability tests and drug release kinetics studies for encapsulated cells.



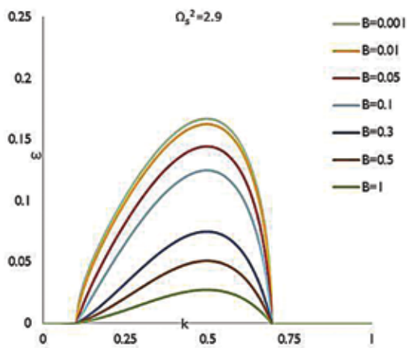
Controlled whipping of an electrified jet in the presence of a coflowing external liquid

2. Investigations into use of polymer nanocomposites as anti-microbial functional coatings:

Preventing or inhibiting the growth of micro-organisms on surfaces is of prime importance in the healthcare and textile industries. In the healthcare industry, proliferation of micro-organisms on medical devices increases the health risk for patients. In the textile industry, growth of microbes on fabrics leads to several undesirable effects such as degradation, foul odour, and health risk. A promising strategy to overcome microbial growth involves coating the surfaces with materials that can provide resistance to microbial colonization. Inorganic nano materials and organic materials with inorganic inclusions are being widely used as anti-microbial coatings. More recently, water-based organic-inorganic nanocomposite materials are finding applications as functional coatings and specifically as anti-microbial coatings. In this project, we are investigating the film formation of organic-metallic latex nanocomposites. Special focus is on the distribution of the metallic filler in the dried films. The antibacterial properties of the obtained films are to be investigated. The synthesis technique is tuned to improve upon the film forming and antibacterial properties of the metallic-based latex nanocomposites.



A blend of polystyrene latex particles and titanium oxide nanoparticles



Stability curves of an electrified liquid jet for various external fluid viscosities.

Publications:

1. Josefa Guerrero, Javier Rivero, Venkata R. Gundabala, Miguel Perez-Saborid, Alberto Fernandez-Nieves, “Whipping of electrified liquid jets”, Proceedings of National Academy of Sciences (PNAS), 111, 13763 (2014).

2. Venkata R. Gundabala, Sergio Martinez-Escobar, Samantha Marquez, Manuel Marquez, and Alberto Fernandez-Nieves, “Celloidosomes via glass-based microfluidics”, J. Phys. D: Appl. Phys. 46, 114006 (2013).

3. Venkata R. Gundabala, Neus Vilanova, and Alberto Fernandez-Nieves, “Current-voltage characteristic of electrospray processes in microfluidics,” Physical Review Letters, 105, 154503 (2010).

Our lab uses Microfluidics and Colloidal Science tools for material synthesis and biological studies.

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Sameer Jadhav

Areas of Interest: Cell Mechanics, Microfluidics, Liposomes, Drug Delivery

Biological cells respond to chemical and mechanical cues in order to accomplish several physiological functions. For instance, stem cell differentiation has been shown to depend upon the structural features, material stiffness and chemical composition of the substrate. Similarly, sperm cells are known to respond to gradients in velocity, temperature and ligand concentrations. Microfluidics technology provides several advantages over traditional methods for analysis and sorting of cells. These include smaller sample size, higher accuracy, fast detection and multiplexing. Our work is focused on applying microfluidics to design bioassays for diagnosis and separation of various cell types based on their morphology, deformability and motility.

Liposomal systems have long been proposed as potential carriers for controlled / sustained and targeted / triggered release of drugs at specific sites of therapeutic interest. We are interested in engineering liposomal delivery systems for macromolecular drugs such as hormones, siRNA and polypeptides. Delivery of such molecules is a challenge due to their size and labile nature. Issues related to stability of the drug-liposome complex, as well as controlled release at the therapeutically relevant sight remain to be addressed.

1. Microfluidic devices to quantitate chemotaxis:

Chemotaxis or cell motility in response to chemical gradients plays a central role in several physiological and pathological processes such as organ development, tissue repair, wound healing, cellular immunity. The cell speeds vary from a few microns per hour, managed by crawling stem cells to several hundred microns per second, achieved by swimming sperm. Microfluidic devices support the generation of stable as well as rapidly switchable chemical gradients. These devices facilitate not only increased precision in measurements on individual cells but also multiplexing capability for statistical estimates of population behavior. We are focused on designing robust microfluidic devices that support stable chemical gradients in the presence of pressure / flow fluctuations. To this end we employ computer simulations to screen and optimize designs that provide superior performance over a range of flow rates. The screened designs are then microfabricated using soft lithography techniques and subjected to experimental validation.

2. Liposomal drug delivery systems:

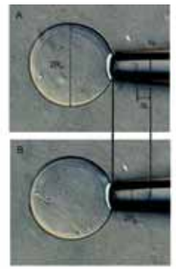
Liposomes are nanometer scale spherical vesicles of phospholipid bilayers and have been used as carriers for delivery of several drugs. While several liposome encapsulated drugs are already on the market, their full potential remains to be realized. Some of the limitations include poor encapsulation efficiencies for certain drugs, difficulties related to site-specific targeting and controlled / triggered release as well as challenges associated with evasion of the reticulo-endothelial clearance as well as lysosomal degradation. Our efforts are concentrated towards optimizing the drug carrier by estimating the effects of drug interaction with the bilayer on liposome stability. To this end, we employ micro-aspiration technique to estimate properties such as moduli for bilayer expansion and bending, bilayer rupture force and bilayer permeability. Several drug-phospholipid compositions are screened for optimal performance parameters such as stability and drug release kinetics.

Publications:

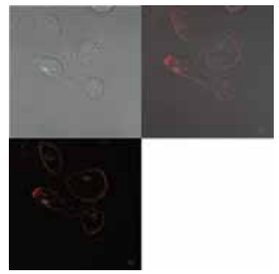
1. YP Patil, S Jadhav, Preparation of Liposomes for Drug Delivery Applications by Extrusion of Giant Unilamellar Vesicles, Nanoscale and Microscale Phenomena, Springer Tracts in Mechanical Engineering (2015), pp 17-29

2. MZ Ismadi, P Gupta, A Fouras, P Verma, S Jadhav, JB Bellare, K Hourigan. Flow Characterization of a Spinner Flask for Induced Pluripotent Stem Cell Culture Application PLoS One (2014) DOI: 10.1371/journal.pone.0106493

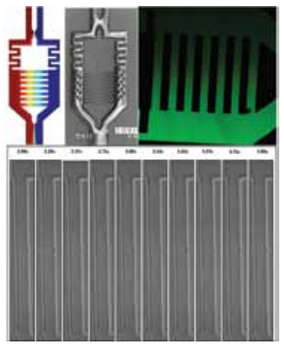
3. V Jayaraj, P Wangikar, S Jadhav "Microfluidic device optimization for cell growth,"IEEE 5th International Nano Electronics Conference (INEC) Singapore (2013) , 157-159.



Micropipette aspiration of phospholipid vesicles to determine membrane properties

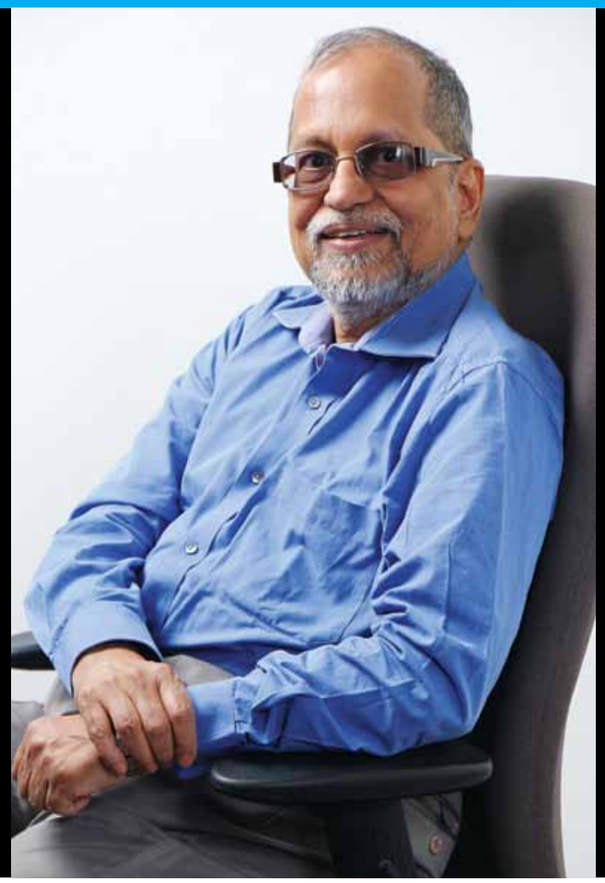


Confocal laser scanning microscopy shows uptake of fluorescently labelled liposomes by MDA-MB-231 breast cancer cells.



Computer simulation and experimental validation of chemical gradient generation and the resulting sperm chemotaxis

Micro- and nano-engineered tools are replacing traditional technologies in the healthcare sector to address issues such as accuracy, cost-effectiveness, ease-of-use and alleviation of patient discomfort.



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Areas of Interest: Interfacial engineering, Electrochemical Engineering, Conducting polymers, Reaction Engineering

Research on interfacial engineering focusses of study of both fundamental aspects and applications of various techniques to stabilize/destabilize interfaces. These include use of polymers to stabilize colloids and emulsions, use of electric field for desalting of crude oil, understating and modifying friction between soft solids sliding on hard surfaces. The fundamental aspects include understanding the role of configurational statistics of polymers chains at the interface as well as interfacial rheology on colloid stabilization, friction, coalescence etc.

Research on electrochemical engineering focuses of modulation of electric field in electrolytic cell in order to achieve high cell performance. The techniques adopted are bipolar electrolysis, polarity switching and pulsing.

Research on conducting polymers involves phenomenological understanding of charge storage capacity and dynamics of conducting polymer films deposited on metal electrodes. These studies will pave ways to design and optimization systems which use conducting polymers as capacitors.

Research on reaction engineering involves study of polynitration reaction, where the role of pi-pi stacking of nitroaromatics on their reactivity.

The focus of the present work is to integrate the equilibrium and dynamic characteristics of various bulk and interfacial phenomena in order to understand behaviour of soft materials in general and interfaces in particular.

1. Conducting polymers:

Conducting polymers possess a property called pseudocapacitance, which make them very attractive as energy storage devices for high power density applications. Dynamics of these polymer electrodes involves a number of charge relaxation modes. We have been able to determine the energy band structure of polyaniline and quantified the capacitance and energy density of these bands. This work would be useful in rational design of conducting polymer-based capacitors.

2. Liquid Emulsion Membranes (LEM):

LEM technique is useful in extracting low concentration of metals/ pollutants from effluent streams. Due to simultaneous extraction and stripping, this technique is practically free from equilibrium limitation, which makes it economically very attractive. A main limitation with this technique is poor stability of water-in-oil (W/O) emulsion. According to our analysis poor integrity of W/O emulsion is caused by Marangoni instability, leading to spontaneous emulsification/ flocculation of oil phase inside water-droplets. Light scattering/interfacial rheology techniques have been used to quantify the spontaneous emulsification and eliminate it by proper choice of surfactant systems.

3. Friction:

Quantification of friction between soft polymeric solids on hard surfaces is important in many applications. We are developing a mathematical model which involves dynamics of adsorption, stretching and desorption of polymer chains dangling from polymer surface in contact with the hard surface. We use the model to quantify static and dynamic friction and stick-slip/stress relaxation phenomena.

4. Open Bipolar Electrolysis:

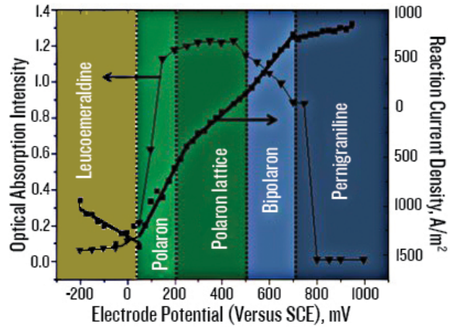
This is a powerful technique for bulk electrolysis. Here a high electric field polarizes electrodes suspended in an electrolyte so that the cathodic and anodic reactions occur on the two sides of each electrode. Thus a large electrode area can be packed in a small space, which makes this technique very attractive for processes involving low conductivity of electrolytes. Our focus is to develop mathematical model for bipolar electrolysis involving single and multiple particles.

Publications:

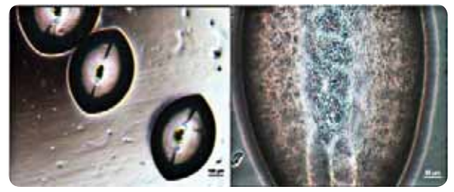
1. Elucidation of band structure of charge storage in conducting polymers using a redox reaction, Asfiya Q. Contractor and V. A. Juvekar, **Anal. Chem.** , 86, pp. 6323–6330 (2014)

2. Analysis of multiparticle bipolar electrolysis using single particle cell model, Rajkumar Patil and Vinay A. Juvekar, **Chem. Eng. Sci., 110,** 72-82 (2014)

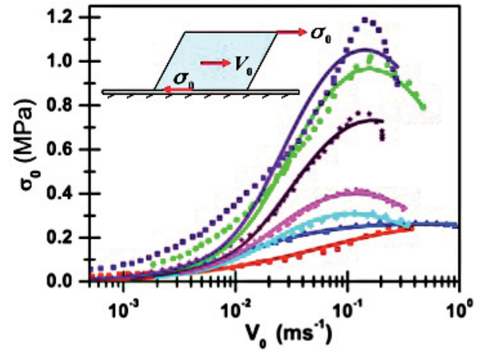
3. Steady of dynamic friction at elastomer-hard solid interface: a model based on population balance of bonds, A.K. Singh and V.A. Juvekar, **Soft Matter,7,** 10601-10611 (2011)



Band structure of Conducing polymer
Picture showing electrochromism (revealed by optical absorption spectroscopy) in polyaniline film associated with its energy band structure. The same band structure is also elucidated through Fe2+-Fe3+ redox reaction in the film.



Spontaneous emulsification
(a)Water drops suspended in paraffin + SPAN 80 (75 mg/ mL oil) Spontaneous emulsification of paraffin inside water drops causes distortion of drops. (b) Flocks of extremely fine paraffin droplets inside water drop



Friction of soft sold sliding on hard surface
Comparison of model predictions with experimental data on dynamic friction stress vs. sliding velocity for varying molecular weights of PDMS

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Devang Khakhar

Areas of Interest: Flow and mixing of powders, Polymers, Liposomes

My research interests lie at the intersection of fluid mechanics and materials with focus in three different areas: Powders, Polymers and Liposomes. The work takes a fundamental approach to understand the systems in depth but in the context of applications. We use experimental and theoretical approaches in all three areas.

Publications:

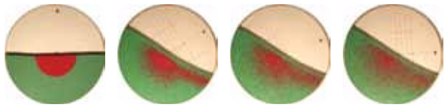
1. A. Tripathi and D. V. Khakhar, Numerical simulation of the sedimentation of a sphere in a sheared granular fluid: A granular Stokes experiment, Phys. Rev. Lett., 107, 108001 (2011).

2. A. Tripathi and D. V. Khakhar, Density difference-driven segregation in a dense granular flow, J. Fluid Mech., 717, 643-669 (2013).

3. S. K. Tiwari, A. Misra and D. V. Khakhar, Benzyl triphenyl phosphonium chloride as an additive for polyvinylidene fluoride: Melt rheology, crystallization and electrical properties, Poylm. Eng. Sci., 54, 2420-2429 (2014).

1. Flow and mixing of powders

Powders, or granular materials more generally, are widely handled and processed in different industries (e.g., pharmaceutical, chemical, ceramic, steel, food and agriculture). The flow of granular materials is quite different from fluids and in the case of mixtures, the particles have a tendency to spontaneously separate out (segregate). We have been working on developing an understanding of the rheology and mixing/segregation of granular materials using experiments, continuum models and particle level DEM simulations. Much of the early work related to flow, mixing and segregation of nearly spherical particles in prototype systems like rotating cylinders and heap flows and was done in collaboration with the group of Prof. J. M. Ottino (Northwestern University). Recent works focus on understanding the special aspects of the flow of non-spherical grains (prolate particles) using DEM simulations and experiments. The objective is to determine the rheology of the flow of such particles. Another problem we have been looking at pertains to the flow during feeding of raw materials into a blast furnace, used in steel manufacture. Detailed experimental studies using high speed videography have been carried out in a model system to measure the flow profile and the segregation as particles flow on the free surface of a heap. Granulation is a process in which a liquid binder is sprayed on a stirred fine powder to cause particles to agglomerate into larger granules, which are easier to handle. Granulation is widely used for products such as detergents, fertilisers, pharmaceuticals, pesticides. We have been studying a subset of the granulation process: the breakage of granules during the granulation process. The work, partially supported by Proctor and Gamble and in collaboration with Prof. Karen Hapgood (Monash University), is based on experiments and DEM simulations.



Mixing of particles in a rotating cylinder. (Hajra and Khakhar, Phys. Fluids, 2005)

Molten PVDF polymer being extruded as a film onto a cast roll. (Mhalgi, Khakhar and Misra, Polym. Eng. Sci., 2007)

Polymers

Our recent work on polymers focuses on the rheology, processing and properties of polyvinylidene fluoride (PVDF), a unique polymer with excellent piezoelectric properties. The is being done in collaboration with Prof. Ashok Misra. An important application of the polymer is for pressure based sensors for a wide variety of uses. The polymer has several crystal phases of which the beta phase is the one with the best piezoelectric properties. Normal processing results in formation of alpha phase crystals, which have no piezoelectric response. Drawing (stretching) of films to four times their length causes a transformation from the alpha to beta phase. We have studied how processing conditions affect the formation of the beta phase as well as the effect of additives on the rheology and dielectric properties of the polymer. The processing is done at a small scale (5 g) as well as at a pilot scale in a continuous extruder system.

Liposomes

Liposomes, or lipid vesicles, are self assembled spherical capsules comprising a lipid bilayer wall with water inside and outside the capsule. Liposomes are widely used for drug delivery and as a simple model for cell membranes. We have been studying the response of such vesicles to external perturbations, in collaboration with Prof. P. Sunthar. In particular, the response to liposome suspensions to ethanol addition has been studied in detail, given the tendency of ethanol to disrupt cell walls. The effect of cholesterol on the response is being studied. Another aspect being considered is the effect of shear flow on the coalescence and breakage of liposomes.

We study different problems related to transport in complex systems (granular materials, polymers and vesicle suspensions) to understand behaviour in simple geometries using experiments and computations and use these insights to build mathematical models.

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Sanjay M Mahajani

Areas of Interest: Reaction Engineering and Catalysis, Process Intensification, Coal and Biomass Gasification

My research revolves around reaction engineering, catalysis and process intensification. The findings are applicable to chemical and energy conversion processes. Some of the important applications being studied are underground coal gasification, biomass gasification for cook-stoves and productions of fuels, fine and petrochemicals. Various process intensification strategies including computational fluid dynamics for clever reactor design, combining reaction and separations (e.g. reactive distillation, reactive chromatography) etc. are investigated for the reactions of interest. This includes both experimental and theoretical studies in catalyst screening, reaction kinetics, separation aspects, conceptual design, process simulation and optimization.

I also work on socially relevant problems wherein, technological interventions are possible. The work involves systematic studies in need identification and technology development meeting the requirement of stakeholders. One such example is conversion of batch jaggery making process to a continuous one to improve product quality and reduce the labor requirement which is otherwise scarce in recent days. The development of process know-how, basic engineering package and pilot plant studies are few of the work elements in this project.

1. Synthesis of Biodiesel:

A various heterogeneous catalysts such as zeolites and metal oxide were developed for the synthesis of biodiesel from vegetable oil. This study mainly involves development of reaction kinetics and using both homogeneous and heterogeneous reactions. The kinetic parameters have been estimated with the help of regression analysis. The esterification and trans-esterification reactions has been performed in packed bed reactor using the selected catalysts to increase the conversion in a continuous mode.

2. Multifunctional Reactors:

Multifunctional reactors combine reactor with other unit operation such as distillation, adsorption, stripping etc. These have several advantages such as reduction in capital cost, increasing selectivity and conversion and decrease in overall cost of the process. Initially, feasibility studies were performed using both experimental and theoretical investigations in several multi-functional reactors such as reactive distillation, reactive chromatography and extractive reactions for industrially important processes (esterification reactions, etherification reactions etc). The mathematical models have been developed and were validated using experimental results. Geometric methods or simulator based design methodologies have been proposed which give good initial estimates of overall process.

3. Underground Coal Gasification (UCG):

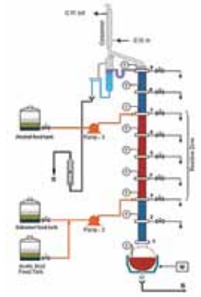
Underground coal gasification (UCG) is a well proven technology which permits access to coal which either lies too deep underground, or is otherwise too costly to be exploited using conventional mining techniques. UCG product gas may be used as a chemical feedstock or as fuel for power generation. Various laboratory scale experiments were performed to determine kinetics in the contest of UCG. A mathematical model of UCG process has been developed and is validated using laboratory scale UCG experiments.

Publications:

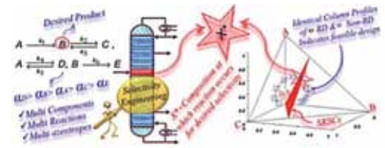
1. Patidar P., Mahajani S.M., Esterification of Fusel Oil using Reactive Distillation - part II: Process Alternatives, Ind. Eng. Chem. Res., 2013, 52 (47),16637–16647.

2. Singh D., Bhoi R., Mahajani S., Ganesh A., Synthesis of Biodiesel from Vegetable Oil Using Supported Metal Oxide Catalysts, Energy & Fuels., 2014, 28, 2746-2753.

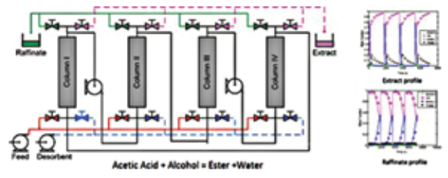
3. Sateesh D., Mandapati R. N., Mahajani S. M., Ganesh A., Aghalayam P., Mathur D. K., Sharma R. K., Laboratory Studies on Combustion Cavity Growth in Lignite Coal Blocks in the Context of Underground Coal Gasification, Energy, 2010, 35 (6), 2374-2386.



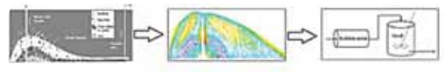
Experimental setup for continuous reactive distillation (CRD)



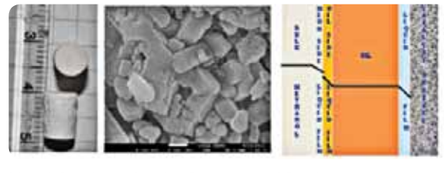
Selectivity engineering with hybrid reactive distillation columns



Experimental setup for simulated moving bed reactor (SMBR)



Schematic of underground coal gasification



Metal Catalysts for the Synthesis of Biodiesel

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Abhijit Majumder

Areas of Interest: Cell-mechanics, microfluidics, soft mechanics

Which comes first, form or function? How different organs get their particular shape during embryonic development? Are cells, the units of life, governed by only genetics and bio-chemicals? Do mechanics and physics play important roles in controlling cell behaviour? If yes, how? How do cells respond to the mechanical properties of their environment? Why do in many diseased conditions, including cancer, these responses get severely modified? These are the central questions of my research group. We work with materials of different mechanical and geometric properties and ask the question how material property of the surrounding environment governs stem cell functioning. Understanding how cells perceive their surroundings and how they react are two essential steps to take our present day knowledge about stem cells from lab to clinic, to design an efficient cell delivery system and scaffolds.

Publications:

1. Vishavkarma, R., Raghavan, S., Kuyyamudi, C., Majumder. A, et.al. “Role of Actin filaments in correlating nuclear shape and cell spreading”, PLOS One, 9, 2014.

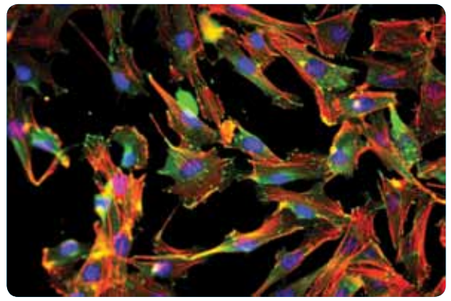
2. Majumder, A.,Mondal, S., Tewari, A and Ghatak, A. “Direction Specific Adhesion Induced by Subsurface Liquid Filled Microchannels”, Soft Matter, 8, 2012.

3. Majumder, A., Dhawan, J., Levy, O. and Karp, JM. “Application of Microfabrication and Microfluidic Techniques in Mesenchymal Stem Cell Research.”, Chapter 4 of “Microfluidic Technologies for Human Health”, Ed By. Demirici U et al. World Scientific, 2012.

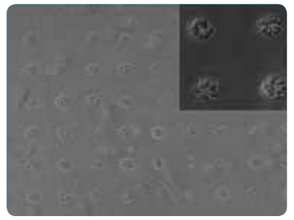
1. Understanding Mechano-sensing and the Role of Mechano-Signals in Determining Stem Cell Fate.

Funding agency: DBT-Wellcome Trust India Alliance, Early-career Fellowship.

The mechanical environment of stem cell niches controls cell fate and cell behaviour. Mechanical cues may be generated by the cells themselves or can be externally applied like flow or vibration. In the past two decades, almost every aspect of cell behaviour including cell survival, migration, cell division, differentiation, and apoptosis have been found to be greatly influenced by mechanical/geometric signals. Irrespective of the nature and origin of a mechano-signal, the mechanism by which such signals impinge genetic programs are not well understood. Although a few key molecular players and pathways have been identified, and the impact of their perturbation have been studied. However, the molecular mechanisms controlling the process of mechano-sensing are still obscure. A consistent database and quantitative model that can connect mechano-signals to the corresponding morphological changes is also a need in the field. My aim is to address some key questions pertaining to mechano-signalling and mechano-sensing. I have chosen to use mesenchymal stem cells (MSC) as my model system considering their multi-lineage differentiation potential and therapeutic value. Specifically, I am interested in understanding how cellular morphology, contractility and mechano-responses are connected, and whether a universal predictor for all kind of mechano-signals and responses exists. I plan to explore the underlying molecular mechanism and to probe the possibility of mechano-transduction via physical deformation of the nucleus. Towards that goal, I propose a two-pronged approach using (a) materials and mechanics (b) cellular and molecular biology.



Two major players in mechano-sensing are actin stress fibres and focal adhesion points. Cells apply contractile force on their surroundings via focal adhesion points (Green dots, vincluin) situated at the end of actin stress fibres (Red lines, actin-phalloidin). Nuclei are shown in blue (DAPI).

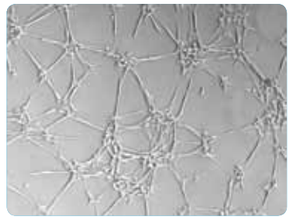


Cells are patterned using micro-contact printing. Using this method size and shape of a cell can be accurately controlled. This helps us in exploring effects of cellular morphology on cell fate.

2. Combinatorial Effect of Bio-Chemical and Mechanical gradient on Cell Migration and Differentiation: A micro-fluidic approach.

Funding Agency: IITB-IRCC, Seed Grant.

Research in recent years has established that both chemical and mechanical signals are crucial in determining almost every aspect of cell fate: cell division, maintenance, differentiation, quiescence and disease. Often, the gradient of a signal plays a more critical role than the absolute concentration of that particular signal. This project aims to explore the combinatorial effect of chemical and mechanical gradient on cell migration and differentiation by developing a novel micro-fluidic based device. At present, availability of experimental assays to study simultaneous gradients/attractants is poor. Even to study single chemical gradient, the choice of a device is limited and each device comes with its own constraints such as additional shear stress on cells for flow-based devices or instability of the gradient for static devices. In this project, we are designing a micro-fluidic device which would be able to create a shear-free, stable and robust chemical gradient. In addition, the device would be compatible with a substrate of gradient stiffness. The chemical and mechanical gradient can be arranged in synch or at any other angle to study the effect of geometry.



Mesenchymal Stem Cells formed network pattern. Although the mechanism of such pattern formation is not completely understood, it is assumed that force interaction play an important role in aligning neighbouring cells. Such pattern formation may give us important clues in understanding morphogenesis.

We are made of cells. And of stars. The Universe outside of us has made the universe inside us.
– L.L. Larison Cudmore, The Center of Life: A Natural History of the Cell (1977), 5.

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Ph.D, Indian Institute of Science, 2009

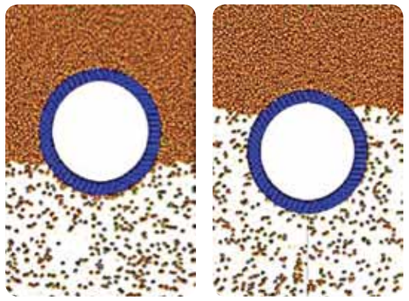
Ateeque Malani

Areas of Interest: Computational Material Science, Wetting and Super-hydrophobicity, Synthesis of Porous Materials, Interfacial and Confined Fluids

Interfacial region is a boundary between different phases or immiscible material and has complex and diverse phenomena compare to bulk system. The analysis of interfacial region has wide ranging application in areas such as, material science, tribology, separation science, catalysis, and membrane science. In my research group, we use multi-scale simulations as a tool to understand fundamental interactions between molecules, their structure and dynamics in the interfacial region, and correlate them with macroscopic properties. Based on these understanding, we design new materials for enhanced wetting, self-cleaning, gas adsorption, separation and lubrications.

1. Wetting and Super-hydrophobicity:

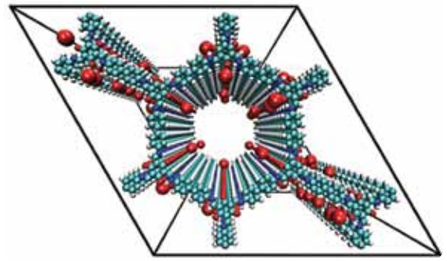
Many natural phenomena, such as, rolling of water droplet on lotus leaf, dryness of bird feather even after immersing in water and skimming of water strider on water surface, are inspiration to prepare biomimetic super-hydrophobic and self-cleaning surfaces. Such surfaces have huge potential applications in variety of areas ranging from chemical industry to food appliances. In the design of such surfaces, the key parameters are the hierarchal design and surface chemistry of materials. We investigate wetting behavior of nano-fibers and nanoparticles using recently developed molecular simulation techniques.



Wetting: Modified fibers to exhibit wetting (hydrophilic) and non-wetting (hydrophobic) behaviors.

2. Design and Synthesis of Porous Materials:

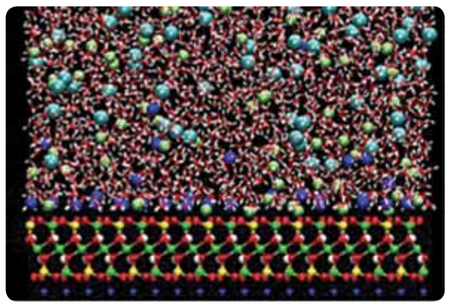
Porous materials are used in many technological industries ranging from petroleum refineries to water treatment plants. The application in wide areas is governed by the internal porous structure of these materials. Theoretical calculations indicate that millions of such materials with unique porous structure can be created; however, only few have been realized in experiments. These novel, yet to be synthesized, material has a great potential in improving existing technologies and application in new areas. We investigate the major road block in finding the routes to synthesize such novel porous materials. We have developed molecular modeling techniques to probe the mechanism at molecular length scale and provide detail kinetic information of porous material synthesis. We are investigating the effect of various processing parameters such as temperature, pressure, concentration of reactant and presence of templating agents.



Porous Materials: Design of novel materials for storage and separation of gases by enhancing porous structure and surface chemistry.

3. Interfacial and Confined Fluids:

Our objective is to obtain fundamental understanding of how a substrate influences organization of interfacial and confined fluid, the origin of forces under nanoscale confinement and the changes in the dynamics of confined fluid. We use Monte Carlo, molecular dynamics and advance techniques to investigate such system. The obtained understanding has huge implications in protein folding, bio-lubrications, adsorption, and separation science.



Solid-Liquid Interface: Structure of liquid (water molecules and ions) near solid liquid interface is responsible for enhanced reaction rates, adsorption, leaching and many more processes.

Publications:

1. A. Malani, A. Raghavanpillai, E. B. Wysong and G. C. Rutledge, Can dynamic contact angle be measured using molecular modeling, Phys. Rev. Lett., 109, 184501 (2012)

2. A. Malani, S. M. Auerbach and P. A. Monson, Monte Carlo simulations of silica polymerization and network formation, J. Phys. Chem. C, 115, 15988 (2011)

3. A. Malani and K. G. Ayappa, Relaxation and jump dynamics of water at the mica interface, J. Chem. Phys., 136, 194701 (2012)

Understanding of the fundamental interactions between molecules at sub-nanometer length scale is essential for optimum design of materials for various applications.

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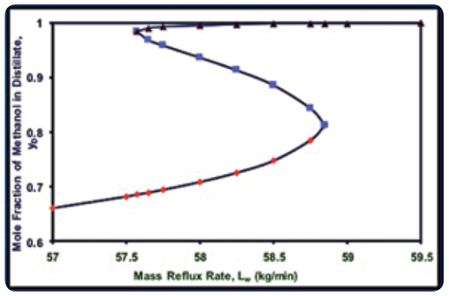
Areas of Interest: Process Simulation & Optimization; Energy Analysis & Process Integration; Separation Processes & Process Intensification; Chemical Product Design.

During the past three decades at IIT Bombay, I have guided research primarily in the area of CAPE (Computer Aided Process Engineering). Some of the areas that I have looked at include Solution multiplicities in multicomponent distillation, advanced distillation technologies for energy reduction, and exergy based conceptual designs of separation systems for improved thermodynamic efficiencies.

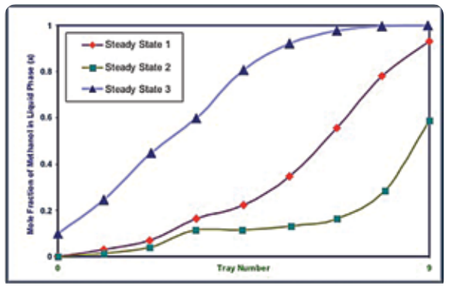
My collaborative research with Prof. Sanjay Mahajani has been in the area of Conceptual designs for selectivity engineering, and feasibility studies for Fischer-Tropsch synthesis through Reactive Distillation.

Chemical Product Design is another area of my recent interest. During the past several decades, in computer aided process design and engineering area, the researchers have given maximum attention to development of algorithms for efficient simulation and Chemical Process Design activity. In recent years, the focus has gradually shifted to Chemical Product Design. A few systematic strategies have been reported in literature in recent years to design environment friendly refrigerants, space materials that can withstand extremely high temperatures, polymers with pre-specified properties, extraction solvents for specific applications, etc. There is need to develop efficient algorithms in this area and my interest is to look into this aspect.

I have provided extensive support to Indian Process Industry in various aspects of Process Systems Engineering through consultancy and customized software development. For the Fertilizer Industry, rigorous mathematical models of various reactors in Ammonia Process (namely, Primary Reformer, Secondary Reformer, Shift Converters, Methanator, Ammonia Converter), and also of Urea Reactor, have been developed and implemented in commercial simulators for several operating plants in India. The mathematical models of ammonia converters have been developed using the building block approach so that these can be easily customized for a variety of configurations. The models have been tested on Topsoe converters (Radial Bed) as well as Casale converters (Axial-Radial beds). For refineries and petrochemical plants, simulation based assistance has been provided through projects on front-end design studies, debottlenecking studies, and design verifications.



Bifurcation Plot for Methanol – Propanol System



Three Steady States for Methanol–Propanol System

Publications:

1. Srinivas S., Mahajani S. M., Malik R. K., Reactive Distillation for Fischer-Tropsch Synthesis: Simulation-based Design Methodology using Aspen Plus, Ind. Eng. Chem. Res., 2010, 49 (20), 9673-9692.

2. Naidu, Y., Malik, R.K. , "A generalized methodology for optimal configurations of hybrid distillation-pervaporation processes", Chemical Engineering Research and Design, 2011, 89 (8), 1348-1361.

3. Hasan, S.U, Mahajani S. M., Malik R. K., Selectivity Engineering with Single-Feed Hybrid Reactive Distillation Columns, Chemical Engineering Science, 2013, 69, 324–334.

The focus of our research is in the key areas of Process Systems Engineering which include applications of mathematical modelling, simulation, design, and optimization techniques for Energy and Process Integration in Petroleum Refineries and Petrochemical Plants.

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Areas of Interest: Colloids, Coarse grain MC simulations, Anisotropic nanostructures-synthesis; Multiphase reactive systems; Carbon capture and Sequestration; Policy issues in higher education, especially, science and technology institutions.

Nanoscale systems:
Advanced colloidal synthesis of complex nanostructures, using bulk and microemulsion protocols; Controlled self-assembly of nanostructures including hierarchical superstructures; Novel templates like worm-like micelles (WLMs) for generating shape anisotropic structures especially of magnetic materials (Co, Ni, Fe3O4); Modeling and simulation of nanomaterial synthesis using Monte Carlo and population balance methods; Applications analysis such as surface plasmon effects in optically active nanoparticles, and hyperthermia efficacies for magnetic particles.

Multiphase reactions:
Carbon capture and sequestration using carbon dioxide absorption in slurries of minerals and industrial slags; Reactive foams and slurries; Aerosol precipitations.

Public policy in higher education:
Effect of admission processes, placement patterns on academic culture; Use of technology in education; Outcome of research funded by state funding agencies.

1. Nanoscale systems:

Rapidly developing fields such as, energy harvesting, advanced materials for aerospace, electronics, medical implants, targetted drug delivery and environmental remediation are potential key application targets for nanomaterials. Synthesis of particles with controlled shape and size is an important objective. It is also important to enable the scale-up of the synthesis processes to larger and industrially viable levels.

Colloidal self-assembly using surfactant systems (as capping agents or as templates) including novel templates like worm-like micellar systems (WLMs) have been used in our lab to obtain a variety of magnetic, semiconducting and transition metal nanostructures. We also strive to understand the evolution of unique structural and crystallographic features in these nanoparticles, in terms of fundamental aspects of nucleation and growth at small scales, both experimentally and theoretically. Applications such as, color properties of nanoparticle suspensions, heating capabilities of magnetic nanostructures have also been investigated.

TEM Nano IRPHA

2. Carbon sequestration:

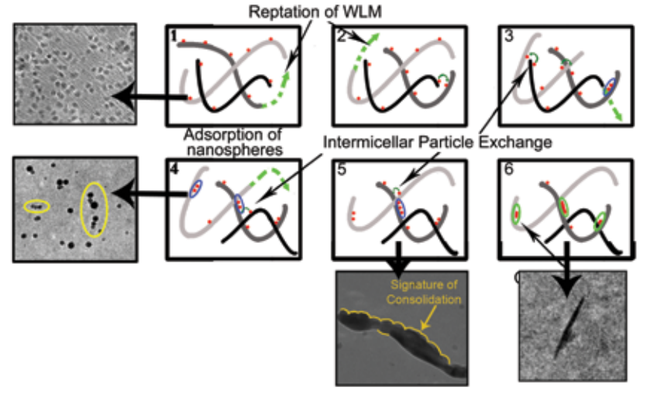
We study the absorption of carbon dioxide into slurries of minerals such as Forsterite and Basalts, and also in industrial slags from steel plants. The objective is to assess the capacity and rates of absorption in batch slurries as well as concentrated pastes, as a function of mineral type, particles size, temperature and pressure.

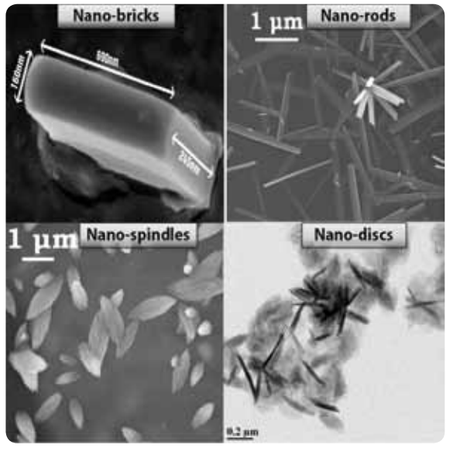
Publications:

1. Seshadri, G., Thaokar, R., and Mehra, A., 2014, ``Optimum size of nanorods for heating application", J. Magnetism Magnetic Mat., 362, 165-171.

2. Chhatre, A., Solasa, P., Sakle, S., Thaokar, R. and Mehra, A., 2012, ``Color and Surface Plasmon Effects in Nanoparticle Systems: Case of Silver Nanoparticles prepared by Microemulsion Route", Colloids & Surfaces A: Physicochem. Eng. Aspects, 404, 83-92.

3. Gupta, V.K.N, Mehra, A. and Thaokar, R., 2012, Worm-like Micelles as Templates: Formation of Anisotropic Silver Halide Nanoparticles", Colloids & Surfaces A: Physicochem. Eng. Aspects, 393, 73-80.





Various nanostructures

The underlying theme of our group is reactive multiphase systems such as colloidal/ surfactant media, and also foams, slurries. An important focus is on characterization and applications of engineered inorganic nanoparticles using a multidisciplinary approach.

Some work is also devoted to the capture and sequestration of carbon dioxide by "fixing" it into minerals and slags

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Areas of Interest: Genomics and Systems Biology, Computational Biology

The general theme of research in my group is to decipher gene transcriptional regulatory networks in microbial and mammalian systems, both at the macroscopic and microscopic levels.

Over the past decade, antimicrobial resistance has emerged as a major public-health crisis, especially in developing countries as more and more clinically relevant pathogens are developing resistance. With the emergence of multi drug-resistant (MDR) and extreme drug-resistant (XDR) *Mycobacterium tuberculosis* strains, there is an urgent need to find novel solutions to counter this resistance. Using *Streptomyces coelicolor* and *Mycobacterium smegmatis* as model systems, we are studying how bacteria modulate their gene expression to respond, adapt and evolve under stress such as that from antibiotics or environmental conditions.

We are also using a combination of cell engineering, process development and mathematical modeling to increase productivity of recombinant therapeutics in Chinese Hamster Ovary (CHO) cells as hosts. Mammalian cells respond to the high load of unfolded proteins in endoplasmic reticulum by the unfolded protein response signaling pathways. The current efforts in the lab focus on the role of this pathway in enhancing productivity.

1. Mechanisms of antibiotic resistance and strategies to counter them.

To identify mechanisms of resistance, our first model system is a non-pathogenic soil bacteria, *Streptomyces coelicolor.* Streptomyces species account for more than two-thirds of all antibiotics. These bacteria are resistant to both endogenously produced antibiotics and that encountered in the soil environment. Our first study explored the multiple mechanisms of resistance exhibited by *Streptomyces coelicolor* against ciprofloxacin, a fluoroquinolone drug. Transcriptomic analysis using whole-genome microarrays suggests that in addition to the up-regulation of target genes, the bacteria counters stress due to antibiotics through up-regulation of efflux pumps and high expression of anti-oxidant genes. Further, growth conditions such as the growth media can modulate gene expression and thus increase the minimum inhibitory concentration of the drug by many folds. Similarly, we have shown that efflux plays an important role in resistance to multiple antibiotics in *Mycobacterium smegmatis.*

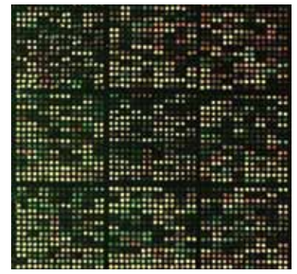
We are also working at ways to counter antibiotic resistance using nano-particles in collaboration with the colloids and nanomaterials group in the department. We have recently demonstrated that a combination of coated iron-oxide (Fe_3O_4) nanoparticles and anti-TB drugs (for example, rifampicin or isoniazid) can lower the minimum inhibitory concentration required to kill *M. smegmatis,* and thus overcome intrinsic resistance. While the nanoparticles themselves are not toxic, a synergistic effect is observed, when used in combination with the drug. We have demonstrated, for the first time, through accumulation and efflux kinetics, that nanoparticles inhibit active efflux of molecules from *M. smegmatis* cells. Further, to mimic clinically resistant strains, we demonstrated that the nanoparticles are effective against laboratory-derived highly drug resistant strains.

2. Cell Culture Engineering:

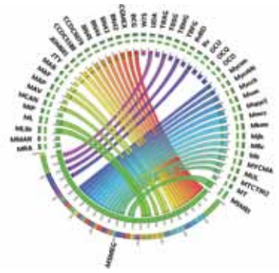
Many recombinant therapeutics are complex glycoproteins for which mammalian cells are the preferred expression systems. With the advent of biosimilars, there is a further need to increase the productivity of these cell lines and accelerate process development. We are investigating the role of the protein secretion pathway in limiting productivity of a panel of CHO cell lines that produce monoclonal antibodies at varying productivity levels from 5 pg/cell/day to 50 pg/cell/day. The experiments are coupled with a mathematical model to guide our efforts to modulate the levels of unfolded protein response UPR pathways genes, using siRNA or chemical inhibitors. Further, we wish to understand the effect of process parameters and reactor configurations on cellular stress and productivity.

Publications:

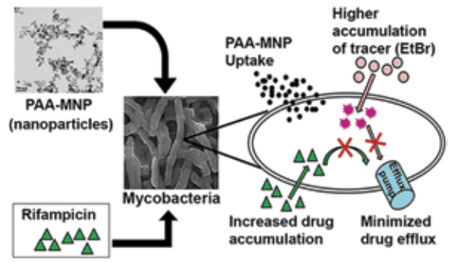
1. Padwal, P., Bandopadhyay, R. and Mehra, S., "Coated magnetite nanoparticles to enhance rifampicin efficacy in *Mycobacterium smegmatis,*" Langmuir, 2014.
2. Patkari, M. and Mehra, S., "Transcriptomic study of ciprofloxacin resistance in Streptomyces coelicolor A3(2)," *Molecular BioSystems;* 9 (12): 3101 – 3116, 2013.
3. Prashad, K. and Mehra, S., "Dynamics of unfolded response in recombinant CHO cells," Cytotechnology, 2014.



A microarray hybridization image showing differentially expressed genes when *Streptomyces coelicolor* cells are treated with ciprofloxacin.



A circos plot showing phylogenetic analysis of Mycobacterial genomes.



Targeting resistant mycobacteria by modulating drug transport through coated nanoparticles.

We employ a multidisciplinary approach using high-throughput omics approaches and computational tools to address problems of industrial and medical significance, such as antibiotic resistance and cell culture engineering.

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Areas of Interest: Liquid and Gas Phase Adsorptive Separations, Industrial Reactor Modeling and Simulation, Attainable Regions, Process Systems Engineering, Process Plant Engineering and Piping Engineering

The Adsorptive Separations, both gas and liquid phase, has been the main area of research. Comprehensive generic simulation models for liquid phase SMB (Simulated Moving Bed) process has been developed and tested for systems of industrial importance such as Parex process for p-Xylene, Molex process for n-paraffins separation from kerosene feedstock. etc. A versatile generic simulation model has been developed for PSA (Pressure Swing Adsorption) process which covers all variations such as VSA, PVSA, RCPSA etc. The model covers all embodiments of hardware such as 2, 3, or multi-bed systems. Extension of the work to cascaded PSA process to handle separations of systems offering low selectivity and which would otherwise not fit the selection criteria for employment of Adsorptive separation, has been proposed and its applicability for Argon separation from Argon-Oxygen mixture has been conceptually demonstrated. The PSA model has been used for Design and Development of a process for natural gas treatment. An industrial unit has been commissioned based on this work.

Present extension of the work involves a hybrid adsorptive separation process where adsorption part is in liquid phase and regeneration is by a gas phase thermal swing. A pilot scale industrial unit for olefin drying will soon be used to generate data to validate this model.

Another area of interest is reactor modelling and simulation. Simulation based optimization/ debottlenecking studies have been used for sulphuric acid manufacturing, hydrogenation, vegetable oil splitting etc. The reactors involved include packed bed catalytic reactors, non-catalytic spray columns, trickle bed reactors etc.

GRM, generalized reactor model, has been developed to cover catalytic and noncatalytic reactors of most industrially important embodiments.

Another interest has been in the area of design and engineering of equipment and piping systems of chemical process industry. A training course on Piping Engineering has been conducted for nearly 25 years for industrial personnel and has benefitted about 10000 working engineers. Another course on Process Equipment Design has been recently released. Both courses are available in contact and on-line mode.

1. Surgeless PSA Process:

An industrial unit to treat about 2 MMSCMD natural gas to remove C3+ components has been designed, engineered, erected and commissioned. It uses model-based control to eliminate the need for surge vessels. The simulation model is used on-line to help the running plant to adapt automatically to changes is feedstock and/or desired product specifications.

2. Leak Detection System (LDS) for fluid flow networks:

A simulation model for gas and liquid flow networks has been developed. PAnORaMA (Piping Analysis, Operations Research and Maintenance Application) is a software application to serve all aspects of in-plant or transportation networks. An online leak detection application based on analysis of live data for fault detection and diagnosis is based on this dynamic simulator. It has seen industrial implementation for the world's largest District Cooling System based on chilled water circulation.

Publications:

1. Mandaliya, D.D., Moharir, A.S., Gudi, R.D. , "An improved Green's Function method for isothermal effectiveness factor determination in one- and two-dimensional catalyst geometries", Chemical Engineering Science: Elsevier, 2013

2. Mhaskar, P. R.; Peter, S. A.; and Moharir, A. S., "Generic Mathematical Model for PSA Process", Chemical Product and Process Modeling: Vol. 7: Iss. 1, 2012

3. Mhaskar, P.R., Moharir, A. S., "Multi-component adsorptive separation: use of lumping in PSA process simulation", Adsorption-Journal of the International Adsorption Society, vol. 17, pp 701-721, 2011

Surgeless PSA: 2 MMSCMD

Certificate Course on Piping Engineering

My students and I work in the areas of liquid and gas phase Adsorptive Separations, Industrial Reactor Modelling and Simulation, Attainable Regions, Process Systems Engineering, Process Plant Engineering and Piping Engineering

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Ph.D, Rice University, 1985

Kannan Moudgalya

Areas of Interest: Simulation environments and simulation methodologies, control system design, affordable labs and virtual labs, open source software, technology assisted learning, collaboration in education, effectiveness of novel pedagogical methods, low cost devices.

We are currently working towards developing a general purpose dynamic simulator by putting together state of the art open source steady state and dynamic simulation packages. In addition to generic software development, this work involves making available theromodynamics, unit operations, solvers and other building blocks. Effective and efficient simulation strategies are explored to get simulations converge in reasonable time.

We are interested in developing affordable laboratory experiments and making them available as virtual labs. We are interested in the real time control issues of virtual labs. We are interested in effectiveness in learning through virtual labs and other technology assisted learning. We are interested in methods of mass and collaborative education and studying their effectiveness. We are interested in development of ecosystems for these activities.

1. Simulation environments and simulation methodologies

We are working on strategies to build general purpose open source simulation environments capable of steady state and dynamic simulation. To this end, we are exploring the possibility of combining DWSIM, a sequential modular simulator and OpenModelica, an equation oriented modelling environment. These two complement each other, and together have the potential to form a good alternative to commercial simulators.

2. Education strategies

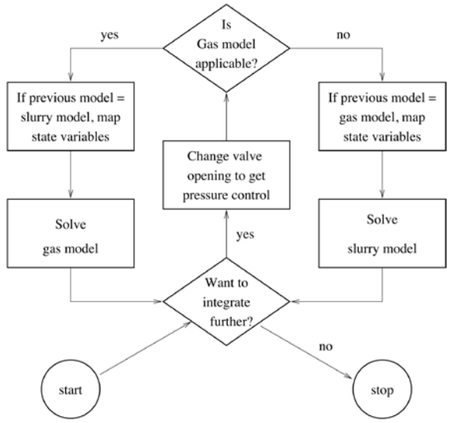
We are working on methodologies to spread good quality chemical engineering education in a big way, through live classes, virtual labs, Spoken Tutorials, SELF workshops, Textbook Companions, Lab Migration and low cost computing devices, such as Aakash and Netbook.

Publications:

1. An Integrated Simulation Environment, by S. Hanumantha Rao, Kannan Moudgalya and K. V. Nori, in Advances in Chemical Engineering, Ed. Y. B. G. Varma and others, pp. 307-312, Allied Publishers, New Delhi, 1996.

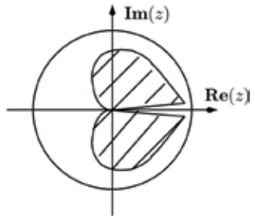
2. A class of discontinuous dynamical systems II. An industrial slurry high density polyethylene reactor, by Kannan Moudgalya and S. Jaguste, Chemical Engineering Science, Vol. 56, 3611-3621, 2001.

3. Digital Control, John Wiley & Sons, Chichester, UK, July 2007. Indian Edition in August 2009.

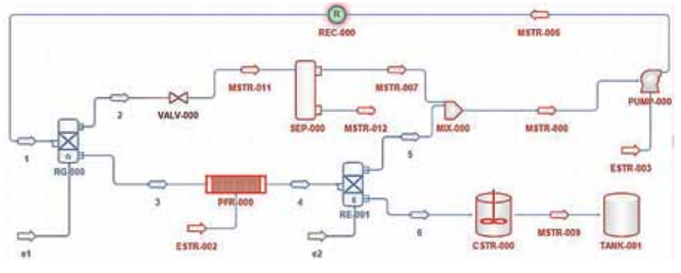


Integrating a discontinuous dynamical system with DASSL

Low cost Single Board Heater System



Desirable region for poles in discrete time control



DWSIM based chemical process simulation on affordable FOSSEE Laptop

We work on modelling, simulation, numerical methods and simulation methodologies, and in the creation of open source simulation environments. To spread these on a massive scale, we are developing appropriate pedagogies and affordable laptops.

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Ph.D, Georgia Institute of Technology, 1998

Hemant Nanavati

Areas of Interest: Polymer Physics and Multiscale Modeling, Bio-resourced and Biodegradable Polymer Systems

Our research has followed a 2-thrust approach, comprising a (1) fundamental understanding of the chemical physics to relate relevant aspects of fundamental molecular structure to physical performance properties of simple homopolymeric systems such as elastomer networks and melts, nanocomposites, and (2) Development of complex value-added structures to first synthesize value-added products such as high crystallinity polymers and nanocomposites.

The objective is to develop a synergy between the results till date in both paths, and to extend our fundamental understanding to more complex polymeric systems such as copolymers, high crystallinity polymers and nanocomposites, highly filled elastomers, dense networks, densely crosslinked networks of polymeric glasses.

The developments in biodegradable polymers need to be consolidated towards making them industrially relevant

The strategy is as follows:

1. Multiscale Simulations of Dynamics (Melts and Highly Filled Elastomers) and Statics (Semicrystalline and Crosslinked Networks) of high crystallinity and nano-filled polymers and networks.
2. Advanced micromechanical experimental methods.
3. Refinement of theory and simulation strategies, based on experiments.
4. Value-addition development in bio-resourced polymeric systems
   a. Scale-up in synthesis of Solid-State Polymerized polylactide and its nanocomposites
   b. Optimization of synthesis to produce superior property products.

Some of the newly developing and ongoing projects include:

1. Molecular Understanding of Deformation of Glassy Thermosets:

Here we examine the deformation of a glassy epoxy, SU-8, which has applications in microelectronics and microelectromechanical systems. We are in the process of understanding the yield behavior at the level of molecular network chains. We are employing advanced experimental tools such as Nanoindentation and Microcompression, and a self-consistent combination of FEA and molecular theory, to examine the entire deformation behavior.

2. Multiscale Modeling of Highly Filled Melts and Elastomers:

Highly filled elastomers find application as solid rocket propellant, as well as in being a rich resource for interesting physics at various scales. The polymeric systems are copolymers, represented in a coarse-grained form, to accurately represent bulk behavior, as well as to form a basis for the framework for interactions with various heterogeneous fillers. The objective is a multi-faceted understanding of such richly endowed systems, with relevant macroscopic properties and applications.

3. Value Addition to Bioresourced and Biodegradable Polymer Systems:

The focus here is scale-up of solid-state polymerization as well as in-situ nanocomposite synthesis of Poly(L-lactic acid) systems. The work is at a practical level, to address typical conditions in India, particularly for scale-up. We are also exploring bioresourced nano-reinforcement for the polymer.

4. Modeling Biopolymers:

Biopolymers such as Dragline Spider Silk, are modeled by a different set of physical and mathematical equations, primarily because of the nature of the units comprising the polymer chains. However, the conceptual similarity in chain structure and physical morphology, enable application of conventional polymer physics concepts, with the modified mathematics superimposed. Indeed, the biophysical aspects such as interaction with water in their natural environment, makes for additional excitement in the investigation.

The aim is to bridge the gap between relevant information from the primary polymer structure and useful, applied performance properties.
We also aim to lead conceptually relevant value-addition and development in bio-resourced and biodegradable polymer systems.

Publications:

1. Hemant Nanavati and Vimal Katiyar, **Method for Producing Lactic Acid Polymers of High Crystallinity and Molecular Weight;** Patent Family: IN 242801, WO 2009007989, US 8697832 B2, EP 2137229, JP 5500451, CA 2681841 A1

2. Ashok Kumar Dasmahapatra, Hemant Nanavati*, and Guruswamy Kumaraswamy*, **Polymer crystallization in the presence of "sticky" additives,** Journal of Chemical Physics, 131(7), August 21, 2009, 074905

3. Kapileswar Nayak, Sushanta Das and Hemant Nanavati*, **Elasticity and Photoelasticity Relationships of PET Fiber Networks by Molecular Simulations,** Journal of Chemical Physics, Volume 128, Issue 1, 2008, 014902

Santosh Noronha

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Ph.D, University of Maryland, Baltimore County, 1996

Santosh Noronha

Areas of Interest: Bioprocess development, Biosystems modeling and data analysis, Healthtech engineering, Education technology

Bioprocess development:
1. Development of recombinant routes for synthesis of chiral intermediates. Methods employed include rational protein engineering for improved biocatalysis and protein overexpression.
2. Development of novel recombinant bacterial, fungal and algal expression systems, all of industrial interest.
3. Isolation of novel enzymes from filamentous fungi.
4. Pathway modification in B. subtilis for accumulation of metabolites.

Biosystems analysis. Understanding, quantitating and manipulating stress responses in microbial systems.
1. Oxidative stress response mechanisms in E. coli and B. subtilis.
2. Nutrient stress responses in filamentous fungi and algal species.

Data analysis: Application of pattern classification and computer-intensive methods for the following problems:
1. Motif identification and tool development for genome analysis.
2. Analysis of biomedical spectroscopic data.
3. Fault detection in (bio)process data.
4. Structure prediction of GPCRs.

Instrumentation-related interests

1. Development of enzyme formulations for treatment of ligno-cellulosic biomass: (on-going):

In this work, we aim to characterize cellulases from a Penicillium strain which is good producer. We also propose to construct an expression system in this fungal strain towards developing it into a large scale producer of homologous and heterologous proteins.
(Sponsor: DBT, 2014-17)

2. Development of bacterial expression systems suited for large scale production of industrial enzymes:

We aim to further improve indigenously developed bacterial expression systems towards obtaining better processes for production of industrial enzymes. Further, we aim to adapt these strains to be better suited as host for whole cell biotransformations. (Sponsors: DBT, 2012-15)

3. Enhancement of Benzaldehyde Biotransformation:

R-PAC is the precursor in the synthesis of ephedrine and pseudoephedrine, alkaloids of considerable commercial value as bronchial dilators and nasal decongestants. This intermediate is commercially manufactured using a whole cell yeast biotransformation of benzaldehyde. We have generated site-specific modified mutants of pyruvate decarboxylase, the enzyme responsible for synthesis of R-PAC, with enhanced selectivity for the condensation reaction involved, resulting in a >50% increase in process productivity. This work was carried out with support from DST and Embio Ltd., and has resulted in a tech transfer. There is further work underway to extend the synthesis pathway to other related products of interest.

4. Development of remote-triggered devices:

This effort is focused on assembling various indigenously developed remote-triggered lab experiments for chemical, biochemical, and control engineers. The objective of this approach is to develop a set of lab experiments consistent with various University curricula, which can be remotely accessed, 24x7, in a robust and secure manner. (Sponsor: MHRD, 2012-17)

5. Development of a low cost arterial tonometry based blood pressure monitoring device:

The objective is to build an arterial tonometry based blood pressure monitoring device (as opposed to conventional oscillometric blood pressure measurement.) Arterial tonometry applies a mild pressure on peripheral arteries (eg. the radial artery) and monitors the pressure pulse waveforms. (Sponsor: IUSSTF/DST, 2014-16)

Publications:

1. Reshamwala, S., Noronha, S. B., “Coproduction of two proteins in Escherichia coli using the promoter region of the divergently expressed curli genes”, J. Biotechnol., 164:121-122, 2013

2. Aggarwal, P.K., Uppada, V., Noronha, S. B., Comparison of pyruvate decarboxylases from Saccharomyces cerevisiae and Komagataella pastoris (Pichia pastoris), Appl. Microbiol. Biotechnol. PMID: 23423327, 2013

An inspection and image storage/transmission device used in screening for cervical cancer

A low cost microfluidics-based POC diagnostic for osteoporosis

Recombinant whole cell enzyme and antigen display systems

I have developed a multidisciplinary approach to bioprocess development, with efforts at genetic, cellular, and reactor-level engineering for production of therapeutics and metabolites. I have also developed an extensive focus on indigenous instrumentation that has extended into the creation of low cost virtual laboratory rigs as well as healthcare devices.

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Ph.D, Indian Institute of Technology, Bombay, 1994

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Areas of Interest: Control relevant modeling of nonlinear dynamic systems, Nonlinear Model Predictive Control, Fault Diagnosis and Fault Tolerant Control, Nonlinear Bayesian State Estimation

Arriving at a model based framework for intelligent monitoring and optimal operation of nonlinear dynamic systems forms the overall goal of my research. The focus of work is on the development of tools for dynamic modelling, nonlinear state estimation, on-line fault diagnosis and synthesis / analysis of nonlinear controllers. Ongoing work is mainly on the following themes:

(1) On-line Model Maintenance and Fault Tolerant Predictive Control: Development of approaches for on-line fault / model parameter identification using mechanistic as well as black-box dynamic models and employing them for adaptive / fault tolerant predictive controller synthesis

(2) Development of linear and nonlinear time series models using generalized orthonormal basis filter parameterization

(3) Development of algorithms for nonlinear Bayesian state estimation (soft-sensing): on-line merging of data with dynamic model predictions for estimating unmeasurable variables / parameters

(4) Grey-box Modelling: Merging mechanistic models with stochastic time series models, noise structure and density estimation from experimental data

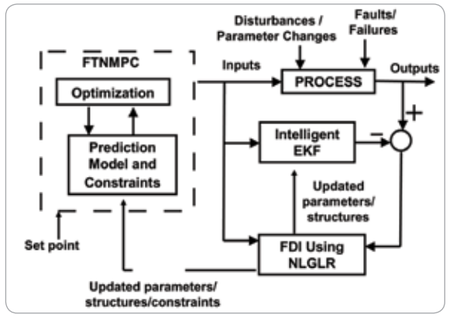
(5) Robust stability analysis of nonlinear state estimators and estimator based nonlinear predictive control schemes using Lyapunov stability analysis framework

Applicability of the tools developed is being investigated through simulation and experimental studies on complex nonlinear systems such as reactive distillation, semi-batch bio-reactors, PEM fuel cell, packed bed distillation and, recently, dc-to-dc power converters.

1. Controller design for simultaneous saccharification and fermentation: (on-going):

The simultaneous saccharification and fermentation (SSF) approach is an industrially important paradigm for the production of cellulosic ethanol. This study proposes to develop and implement a low cost adaptive model predictive control framework which efficiently manages multi-rate measurements, environmental perturbations and feed-grade transitions.These goals will be achieved by integrating exit gas analysis based sensors (ethanol, O2, CO2) and an online FT-NIR spectroscopy system (for characterizing the hydrolysis products) into the proposed control framework.Identifying the extent to which an instrumented and controlled process would reduce dependency on enzyme costs, as well as facilitate robustness to process fluctuations is one of the main focus of the project.

(Sponsors: Dept. of Bio-Technology, Govt. of India)

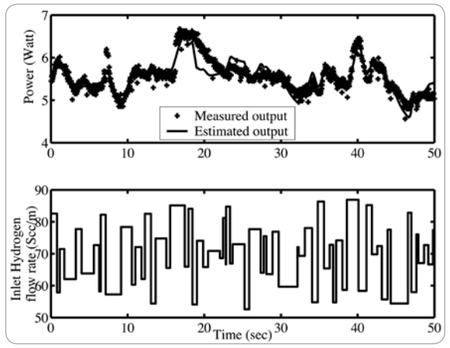


Schematic Representation of Fault Tolerant Nonlinear Model Predictive Control (FTNMPC)

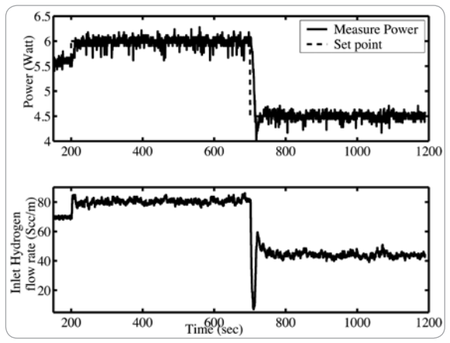
2. Development and Evaluation of nonlinear data-driven models suitable for nonlinear model predictive control of a Fluidized Bed Reactor (FBR) in PolyEthylene (PE) manufacturing process (2007-10):

This work explored possibility of developing nonlinear data driven block oriented black box models with Wiener / Hammerstein / Wiener - Hammerstein structurefor capturing nonlinear dynamics of a Fluidized Bed Reactor (FBR) system. These models were parametrized using generalized orthonormal basis filter (GOBF). In particular, design procedure was evolved for generating plant friendly input excitation signal to obtain the input-output data such that the identified black box model reveals salient nonlinear features of FBR system. Modeling studies indicated that GOBF-Wiener models were able to capture features of steady state and dynamic nonlinearities satisfactorily. Multiple nonlinear model based framework was also investigated for modeling grade transitions in the FBR system.

(Sponsors: Honeywell Technology Solutions Lab, Bangalore)



PEM Fuel Cell Experimental Setup: Dynamic Model Validation



PEM Fuel Cell Experimental Setup: Servo Control using Nonlinear IMC

Publications:

1. Bavdekar, V. A. and Patwardhan, S. C., "Development of Grey Box State Estimators for Systems Subjected to Time Correlated Unmeasured Disturbances", Journal of Process Control,22, 1543– 1558, 2012.

2. Huang, R.,Patwardhan, S. C., Biegler, L. T., Robust nonlinear model predictive control based on discrete nonlinear extended observers. Journal of Process Control, 22, 82– 89, 2012.

3. Patwardhan, S. C.,Narasimhan, S., Prakash, J., Gopaluni, R.B., Shah, S. L., "Nonlinear Bayesian State Estimation: Review And Recent Trends", Control Engineering Practice, 20, 933–953, 2012.

Focus of my research is on development of a model based framework for optimal operation of nonlinear systems. Tools for nonlinear time-series modeling, Bayesian state estimation and fault tolerant model predictive control are being developed and validated on variety of systems through simulation and experimental studies.

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M.S, State University of New York, 1982

Sandip Roy

Areas of Interest: Risk-based Process Safety Management, Cultutral Aspects of Process Safety Management, Supercritical Fluid-based Processing

Introduction to Research Programs:

1. Models for risk-based management of maintenance of chemical process are being developed. They include approaches that involve stochastic modeling of failure processes, fuzzy logic for multi-criteria decision-making for maintenance programs for process plants. A methodology of risk-based optimization of process plant layout that incorporates domino effects is being developed. The effect of inclusion of cost of rehabilitation in the overall objective function as well as compliance with universal regulatory criterion on public individual risk as well as societal risk is being explored. Additionally, work is underway to develop a methodology to predict Public Individual and Societal Risk acceptance criteria for based on economic theory that use Life Quality Index as a decision-making parmater.

2. While adoption of process safety management systems in the global process industry has been intensifying losses continue to occur, owing largely to human factors. The present research explores the possible role of fundamental national cultural attributes in determining workplace behaviour and thus ultimately the safety culture of an organization.

3. A variety of supercritical and subcritical carbon dioxide-based micronization processes are being studied through experiments and model development. Examples include: SAS, GAS, PPRGEL, etc. The goal of this research program is to evolve generalized models that may help predict and therefore engineer particles of a desired size.

Over the recent years our group has been focusing on a number of industry-funded research projects that involve supercritical fluid-based processing. These broadly maybe subsumed in the areas of: micronization of pharmaceutical actives, dyeing of fabrics. In the former category protocols for micronization of a variety of pharmaceutical actives have been developed along with theoretical models for prediction of particle size as a function of process parameters. The models combine thermodynamic and kinetic aspects of the process and make use of classical and modified theories of homogeneous and heterogeneous nucleation. The simulations executed using these models indicate that the models are amenable to use for obtaining optimal process conditions for obtaining a desirable range of particle size. In the second category, a range of fabrics and dyes have been considered for experimental study of uptake of dyes under supercritical conditions. The processes so developed aim to replace traditional, aqueous-phase dyeing which generate considerable amounts of waste water, which cannot be recycled cost-effectively. Unique protocols for pre-treatment and post-treatment of the fabrics have been developed to ensure appropriate levels of dye uptake and retention. The experimental work has furthered the general understanding of the underlying dye transport and adsorption processes in supercritical fluid media.

Publications:

1. Ghosh, D. and Roy, S, "A Decision-making Framework for Process Plant Maintenance", in *European Journal of Industrial Engineering,* 4(1), 78, 2010.

2. Mriganka Mondal, Sandip Roy, and Mamata Mukhopadhyay, *Ind. Eng. Chem. Res.,* 2015, Vol. 54 (13), pp. 3451–3461, DOI: 10.1021/ie504960u

3. A. Sengupta, D. Bandyopadhyay, S. Roy, C.J. van Westen, A. van der Veen, Challenges for introducing risk assessment into land use planning decisions in an Indian context, *J. Loss Prevention in Process Industries* (2015), doi:10.1016/j.jlp.2015.10.007

SCF based Particle Precipitator

SCF Extraction Pilot Plant

SCF Micronizer

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Ph. D, University of Illinois at Urbana–Champaign, 2010

Supreet Saini

Areas of Interest: Microbial evolution, dynamics of biological systems, bacterial pathogenesis

Living cells are constantly monitoring their environment, and appropriately modulating their behaviour. This modulation happens via precise organization of cellular functionalities over many scales (for example, DNA sequence, formation of operons, mRNA structures, regulatory networks, signal transduction, and inter- & intra-specie communication).

Related to this, our group is interested in two broad questions: first, what are the properties (and advantages) of naturally occurring regulatory networks in microorganisms over alternate designs, and second, what are the dynamics and statistics of the process of evolution of an optimal regulatory design for a cellular function? These questions motivate us to study dynamics of biological processes and systems, and try to decipher the design principles that give them their particular shape and structure.

Toward this end, we study model systems in bacteria – including those related to control of virulence in Salmonella, E. coli, and Bordetella; emergence of antibiotic resistance in E. coli; and metabolism & its control in E. coli, Zymomonas, and Clostridium.

1. Control of virulence programs in pathogenic bacteria.

Infectious bacteria are able to modulate gene expression appropriately in precise environmental niches leading to infection. A number of factors - including those related to movement (flagella), attachment (fimbriae), resistance to antibiotics (via intrinsic genes, or horizontally acquired genes), infection (secretion systems), toxicity (toxins) – need to be expressed in at the right locales, at the right time, and in right amounts for successful infection. The relative timing of switching these systems "On" (and "Off") of these factors is critical in enabling the bacterium to cause infection. Using Salmonella, Bordetella, & pathogenic E. coli, our group tries to understand the design principles of control of multiple processes in bacterial pathogens.

2. Evolution of Gene Regulatory Networks in microbial populations.

Microorganisms have evolved complex and highly interconnected regulatory networks to grow and divide in their niche. How do these structures evolve over time? And what are the dynamics and statistics associated with this evolution of regulatory networks? In this research, we are trying to answer these questions by "reverse engineering" genetic networks in the common bacterium E. coli and monitoring dynamics and statistics of evolving networks under different selective pressures.

3. Metabolic Engineering.

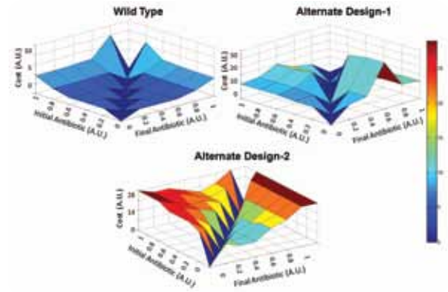
As part of their general metabolism, microorganisms produce a number of chemicals of value. Recent years has seen several efforts in engineering the natural circuitry in microorganisms and try and produce (or optimize production of) value chemicals as part of organisms metabolism. This process involves introduction of foreign genes which encode for non-native enzymes, or "tweaking" the timing and level of expression of naturally occurring enzymes. Our interest in this area lies in understanding how organisms adapt and respond when regulatory and metabolic structures that have evolved over millions of years, are fiddled with? More precisely, we are working towards understanding if there are "rules" which dictate the mutations that these synthetically engineered microorganisms (or wild type strains) acquire when exposed to a particular environment.

Publications:

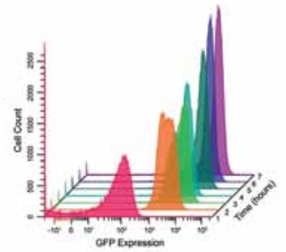
1. Revisiting Demand Rules for Gene Regulation. MK Prajapat, K Jain, D Choudhury, GS Chaudhary, S Saini. bioRxiv (2015) doi: http://dx.doi.org/10.1101/014142

2. Elementary mode analysis reveals that Clostridium acetobutylicum modulates its metabolic strategy under external stress. M Kumar, S Saini, K Gayen. Molecular BioSystems (2014) 10(8):2090-105

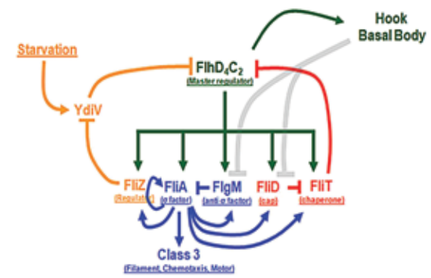
3. Role of feedback and network architecture in controlling virulence gene expression in Bordetella. MK Prajapat, S Saini. Molecular BioSystems (2013) 9(11), 2635-2644.



Cost-benefit analysis in E. coli cells exposed to rapidly varying antibiotic concentrations for wild-type and alternate designs.



Gene expression dynamics at a single-cell resolution for membrane porins in E. coli.



Regulatory network driving flagellar biosynthesis in Salmonella.

Due to their ability to modulate reactions taking place at any particular time, living cells are remarkable chemical reactors. Our group is interested in understanding the "rules" of the evolutionary process through which bacteria develop this property.

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Ph.D, The University of Texas, 2009

Arindam Sarkar

Areas of Interest: Fuel cells, electrochemistry, electrocatalysis, nanomaterials

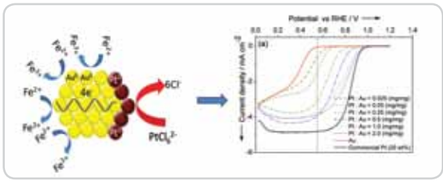
Fuel cells are expected to revolutionize the transportation sector since **Sir William Robert Grove** converted the chemical energy of hydrogen and oxygen directly to electrical energy in 1840. However, the limitations of catalysts have hindered widespread applications. We strive to develop better catalysts and fundamentally understand how they affect reactions.

A major part of our studies revolve around the effect of electrical energy in terms of voltage and current to a chemical reaction and vice-versa. As with temperature, application of voltage changes the kinetics of chemical reactions, albeit to a far greater extent.

Another area of our research focused on synthesis and electrochemical properties on nanomaterials especially "core-shell" nanoparticles.

1. Electrochemical oxygen reduction on platinum sub-monolayer electrocatalysts

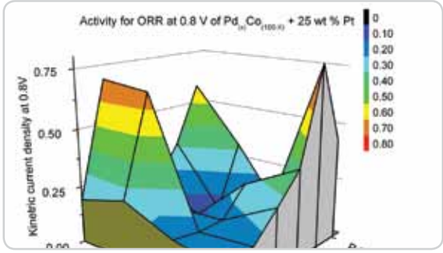
Project Summary: The project deals with electrochemical oxygen reduction on platinum sub-monolayer "core-shell" electrocatalysts. Platinum sub-monolayer electrocatalsyts are being synthesized by copper underpotential deposition on various noble metal nanoparticles (Pd, Au, Ir etc.) supported on carbon and afterward displacing the copper atoms by platinum atoms. The project would also study the feasibility of using electrochemical techniques to determine the surface concentration of bimetallic nanoparticles. Further, the activity for oxygen reduction reaction will be determined for each samples using a rotating disk electrode (RDE) in acidic media to elucidate the effects of surface concentration and the core.



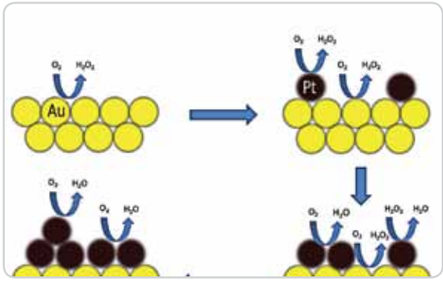
Electrochemical oxygen reduction behavior of selectively deposited platinum atoms on gold nanoparticles

2. Electrochemical oxidation of polyols for electrical power and electro-synthesis of valuable chemicals

Project Summary: The project deals with development and synthesis of electrocatalysts for generation of electrical power and electro-synthesis of valuable chemicals from electrochemical oxidation of low molecular weight polyols (ethylene glycol ($C_2H_6O_2$) and glycerol ($C_3H_8O_3$)). The primary objective would be to (a) synthesize several "core-shell" noble metal based electrocatalysts and (b) evaluation of their activity for oxidation of low molecular weight polyols for power generation. The project would also explore the selectivity of different catalysts towards electro-synthesis of high value chemicals.



Mapping activity of ternary alloys with composition and temperature



Transition of oxygen reduction reaction from 2 electrons pathway to 4 electrons pathway.

Publications:

1. Sarkar, A.; Kerr, J. B.; Cairns, E. J. Electrochemical Oxygen Reduction Behavior of Selectively Deposited Platinum Atoms on Gold Nanoparticles. ChemPhysChem 2013, 14, 2132–2142.

2. Sarkar, A.; Zhu, X.; Nakanishi, H.; Kerr, J. B.; Cairns, E. J. Investigation into Electrochemical Oxygen Reduction on Platinum in Tetraethylammonium Hydroxide and Effect of Addition of Imidazole and 1,2,4-Triazole. J. Electrochem. Soc. 2012, 159, F628–F634.

3. Sarkar, A.; Manthiram, A. Synthesis of Pt@Cu Core–Shell Nanoparticles by Galvanic Displacement of Cu by Pt4+ Ions and Their Application as Electrocatalysts for Oxygen Reduction Reaction in Fuel Cells. J. Phys. Chem. C 2010, 114, 4725–4732.

The application of electrical energy to a chemical reaction instead of heat energy opens exciting possibilities and paves way for newer materials and processes.

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Jyoti R Seth

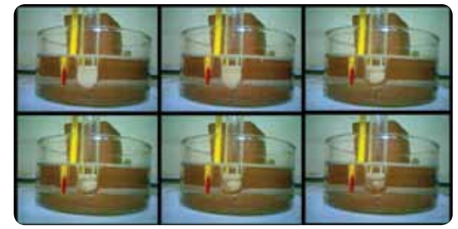
Areas of Interest: Soft Matter, Rheology, Suspensions, Bio-refining

We study how interfacial forces impact the dynamics of complex fluids such as suspensions, emulsions, foams, micro-emulsions, polymers and glasses. These are already crucial for industrial processes and products due to their peculiar rheology and flow characteristics. But we are now in an era where industries must maneuver through quick transitions in technologies under restricting resources, laying stress on novel materials that tailor to a purpose with a specific property. Through a combination of experiments and theoretical models we create the desired characteristics by using fundamentals of solid mechanics, hydrodynamics, surface phenomena and statistical thermodynamics. We rely on experimental techniques of imaging, diffraction and scattering, rheometry and use computational techniques such as molecular dynamics and finite element methods. Our goal is to design materials to meet benchmarks such as targeted response, guided transport in a medium, stimulus dependent rheology, etc., relevant in consumer goods, pharmaceutical, polymer, petroleum and other industries.

Our work covers two fundamental areas: rheology of complex fluids such as suspensions and glassy composites; and dynamics of soft interfaces:

1. Use of microemulsion glasses as templates for nanostructured composites:

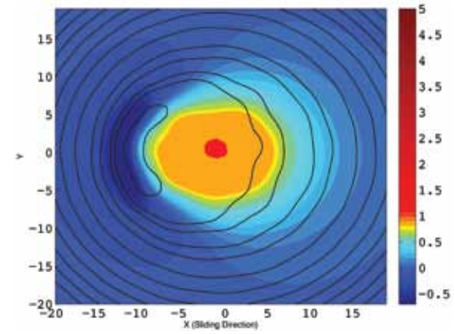
Complex glasses formed from micro-emulsions are a relatively recent discovery and provide an elegant way to arrest the self-assembled microstructure. Mixture of sugars form the polar component for the micro-emulsion that undergoes vitrification a little above room temperature, paving way to prepare stable arrested solid micro-emulsions resistant to phase separation or structural transformations. An experimental procedure has been developed to prepare such "complex glasses" from the one-phase bicontinuous micro-emulsions. We are exploring use of these nanostructured glasses as templates for formation of polymer membranes with nano-pores and other functionalized composites.



Transition from opaque dispersed sugar-surfactant mixture in oil in to clear one phase. We observe that the mixture spontaneously self-assembles in to a microemulsion. The above figure is for sample at 75^{o}C in a silicon oil bath with each frame taken at 2 min intervals.

2. Suspensions of anisotropic particles:

Because of their aspherical shape, anisometric particles have a low percolation threshold and form a space-percolating network at low volume fractions. We study how the self-similar structural hierarchy is generated when suspensions of anisotropic particles are prepared through the process of crystallization. Suspensions containing fatty acids and their triglycerides are quintessential examples of crystalline systems where dynamics of crystal growth, aggregation and resulting suspension behavior can be studied. Further, certain additives, even in minute quantities, can influence the choice of polymorph and/or face dependent growth kinetics of crystals. This proves critical for industries where rheology of the suspension is critical for performance, stability and perceived quality.



Superimposed height (lines) and pressure (filled) contours for lubrication flow between a rough particle sliding over a smooth wall.

3. Lubrication flow near Soft and Rough Contacts:

We are studying lubrication flow dynamics around naturally occurring rough topographies. We solve for deformation of elastic surfaces of different roughness along with the Reynold's equation for lubrication flow in between and around asperities. Surface and pressure profiles, and the effective drag and lift forces experienced by the soft body compare against experimental measurements made with rough elastic substrates. The model is being used to extend our understanding of lubrication flow of non-Newtonian fluids between soft confinements.

Publications:

1. Seth J. R., Locatelli-Champagne C., Monti F., Bonnecaze R. T., and Cloitre M., "How do soft particle glasses yield and flow near solid surfaces?" Soft Matter, 8, 140-148 (2012).

2. Seth J. R., Mohan L., Locatelli-Champagne C., Cloitre M. and Bonnecaze R. T., "A micromechanical model to predict the flow of soft particle glasses," Nature Materials, 10, 838–843 (2011).

3. Seth J. R., Cloitre M., Bonnecaze T. R., "Influence of short-range forces on wall-slip in microgel pastes", Journal of Rheology, 52, 1241-1268 (2008).

My group is innovating towards creating tailor to purpose materials. We use modeling and simulation tools to solve for material composition toward desired rheological or functional properties.

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Yogendra Shastri

Areas of Interest: Bioenergy, Sustainability, Optimization, Supply Chain

Achieving sustainable development by balancing the long-term economic, environmental, and social objectives is one of the most complex scientific problems of this century. Our group focuses on developing and implementing systems theory based tools such as modeling, optimization and control, which enable the integration of inherently multi-scale, multi-disciplinary phenomenon and provide decision making tools for sustainable development. The specific areas of application include microalgal and lignocellulosic biofuels, post-harvest loss minimization, municipal solid waste management, and natural resource management. We are developing large scale optimization models for optimal synthesis of integrated microalgal and lignocellulosic biorefineries. We are also optimizing the designs of novel processes such as reactive flash volatilization and hydrothermal liquefaction of microalgae. We are focusing on designing inherently resilient and optimal biofuel process systems, including processes and the associated supply chains, to handle uncertainties and fluctuations. The research also finds application in minimization of losses of perishable products such as grains, fruits and vegetables. We also work on developing multi-scale agent-based models to study the sustainability of large and complex systems so as to provide policy recommendations for industries, societies, and the government. Apart from making novel methodological and conceptual contributions, work in our group is also driven by the underlying theme of addressing issues relevant to India.

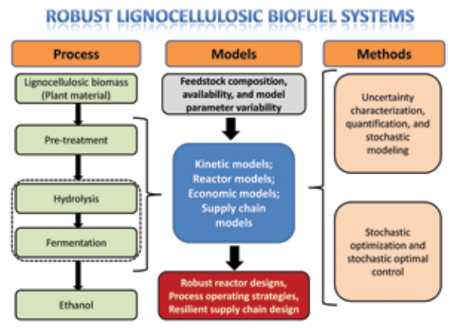
1. Optimization of integrated algal biorefinery

Development of an integrated biorefinery that produces biofuels as well as low volume, high value co-products could make microalgal biofuels techno-economically feasible. The synthesis of such an integrated biorefinery is challenging due to multiple pathways, products, and design specifications. Our work addresses this challenge by performing model-based superstructure optimization. Important stages in biodiesel production, namely, growth, harvesting and dewatering, lipid extraction, and transesterification are modelled. For each stage, several potential options are considered. The objective function is minimization of the net annualised life cycle cost of biodiesel production for a fixed annual demand. It is a mixed integer linear programming (MILP) problem, which is modelled in GAMS and solved using the CPLEX solver. The model will be extended further to consider the production of value added co-products.

Sustainability paradigm balancing economic, environmental and social objectives

2. Stochastic optimization of lignocellulosic biofuel system

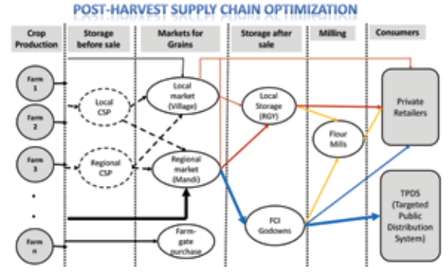
Biochemical processing of lignocellulosic feedstock into fuel and value added products is impacted by various static and dynamic uncertainties such as feedstock quality, supply, and process efficiency. We are developing and implementing efficient stochastic modeling and optimization approaches for robust process design in the presence of these uncertainties. We are primarily focusing on studying the pre-treatment and hydrolysis steps of the process. We have developed detailed reaction kinetic models from literature for these two processes and have conducted stochastic simulations to quantify the impact of uncertainties. We have performed global sensitivity analysis on these models to identify key model parameters.



Design and management optimization of lignocellulosic biofuel systems: Processes, models, and methods considered in our work

3. Post-harvest loss reduction in agricultural

Grains such as wheat and rice suffer extensive losses along the post-harvest supply chain in India. Minimization of these losses is necessary yet challenging due to the highly complex nature of the supply chain. This work aims to determine the best combination of alternatives using optimization theory. We have developed a large scale optimization model for the post-harvest supply chain of wheat in India. The decision variables are the supply chain network links, flow of wheat along these links, and location and size of storage facilities. The objective function is minimization of the total cost and post-harvest losses.



Post-harvest supply chain of wheat in India: Optimization model scope and components

Publications:

1. A. Soman and Y. Shastri. Optimization of novel photobioreactor design using computational fluid dynamics. Applied Energy, 140: 246-255, 2015.

2. S. Sen Gupta, S. Bhartiya, and Y. Shastri. The practical implementation of algal biodiesel: Challenges and potential solution. CAB Reviews: Perspectives in Agriculture, Veterinary Science, Nutrition and Natural Resources, 9(20): 1-12, 2014

3. Y. Shastri, Z. Miao, L.F. Rodriguez, T.E. Grift, A.C. Hansen, and K.C. Ting. Determining optimal size reduction and densification for biomass feedstock using the BioFeed optimization model. Biofuels, Bioproducts & Biorefining, 8(3): 423-437, 2014.

Sustainable development is the development that meets the needs of the present without compromising the ability of the future generations to meet their own needs.
– Our common future, Brundtland Commission (1987)

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Ph.D, Indian Institute of Science, 2002

P Sunthar

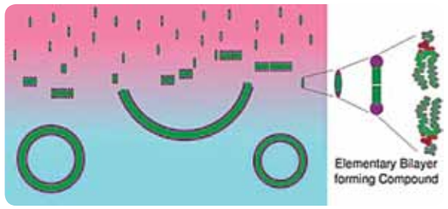
Areas of Interest: Vesicles for drug delivery, Computerised evaluation systems

Lipid vesicles or liposomes are biologically friendly carriers of drug molecules and genes to targeted tissues in a body. Our research focuses on methods to synthesise and encapsulate vesicles in a way that is scalable and possibly carried out at the point of care. We look at methods of synthesis of vesicles from a solution phase.

Grading of knowledge, reasoning ability, and skills for a populous country is faced with difficulties of accuracy, consistency, confidentiality, and logistics. We are developing methods to computerise most of these steps in order to develop an examination system that can be scaled up without compromises in any of the above challenges.

1. Stationary Phase Inter-diffusion (SPI):

Laboratory methods to produce unilamellar vesicles of a definite size either rely on an external energy input (such as sonication or extrusion), using multi-component systems (such as catanionic, lecithin+bile, etc.) or by inducing a spontaneous curvature through certain molecules. We have developed a method where lipids spontaneous assemble from a solution phase that results in predictable diameter vesicles. In this method stationary phases (one containing the lipid and other being aqueous) is brough into contact without any advective mixing. The time of synthesis of liposomes by this method can be made as low as 15 minutes. This method is being further improved to be used in portable devices for point-of-care drug delivery and in industrial systems for bulk production of vesicles.



Self-assembly of vesicles in SPI method

2. Anomalous diffusion in nanoparticle suspensions:

It is observed that nanoparticles enhance mass transfer of solute particles. While there have been many beliefs around what causes this apparent increase, there is no fundamental theory or experimental evidence to back any of them. Our group is designing elementary experiments to isolate various possible interferences and factors that are reported in the experiments of enhanced transport. Our hypothesis of the phenomenon is around a driven motion of the nanoparticle itself, which inturn leads to a flux of the solute. There are various known and well understood motions of colloidal particles which are being tested.

3. Distributed Digitised Answerbook Evaluation:

For a populous developing country such as ours, there is a need to develop indigenous solutions for examination systems, matching the quality of the best solutions available in the market. The science and engineering behind these technologies are well known. It is therefore possible to develop software solutions using open source tools, and make available open source solutions which can be further developed and maintained by the community of users. We are developing a language neutral software system for on-screen evaluation of digitised paper based answer booklets, associated answer book design, printing and post-exam booklet handling standards and protocols, marking statistics and MIS for an unbiased, secure, and error-free evaluation.

Publications:

1. Sunthar, P and Phapal, Sopan (2015), “Rapid Spontaneous Assembly of Single Component Liposomes”, arXiv:1501.00541 [cond-mat.soft]

2. Pan, S., Ahirwal, D., Nguyen, D.A., Sridhar, T., Sunthar, P., Prakash, J.R. (2014), “Viscosity Radius of Polymers in Dilute Solutions: Universal Behavior from DNA Rheology and Brownian Dynamics Simulations”, Macromolecules, 47, 7548-7560.

3. Pan, S., At Nguyen, D., Sridhar, T., Sunthar, P., Ravi Prakash, J. , (2014) “Universal solvent quality crossover of the zero shear rate viscosity of semidilute DNA solutions”, Journal of Rheology, 58, 339--368.

Taking colloidal physics to affordable healthcare.

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Akkihebbal K Suresh

Areas of Interest: Multiphase reaction engineering, Interfacial polycondensation, transport in nanofluids, Solid-solid reactions.

Our group's research efforts are focused on multiphase transport-reaction problems. Applications of industrial interest include liquid phase oxidation of hydrocarbons and oxygen-containing compounds, intensification of absorptive processes for carbon capture, solid-phase transformations of metal oxides such as calcia-alumina systems and Membrane synthesis for gas-separation and reverse osmosis (details below). The attempt in all cases is to understand the mechanisms involved so that the systems can be exploited better in terms of efficiency and productivity. A somewhat more recent interest has been in the areas of alternative medicinal systems such as Ayurveda and homeopathy, where again, we attempt to understand the physicochemical and biological bases for the action of claimed therapeutical principles.

Publications:

1. S. Komati and A.K. Suresh, "Anomalous enhancement of interphase mass transfer rates by nanoparticles: Effect of magnetic iron oxide on gas-liquid mass transfer", I&EC Research, 49(1), 390-405 (2009).

2. R. Amaresh, M. Pathak and A.K. Suresh (2014), " Kinetics of solid-solid reactions: Influence of the number of contact points", I&EC Research, 53(29),11659-11667 (2014).

3. P.S. Chikramane, D. Kalita, A.K. Suresh, S.G. Kane, J.R. Bellare, "Why extreme dilutions reach non-zero asymptotes: a nanoparticulate hypothesis based on froth flotation", Langmuir, 28(45), 15864-15875 (2012).

1. Intensification of mass transfer processes using nanofluids.

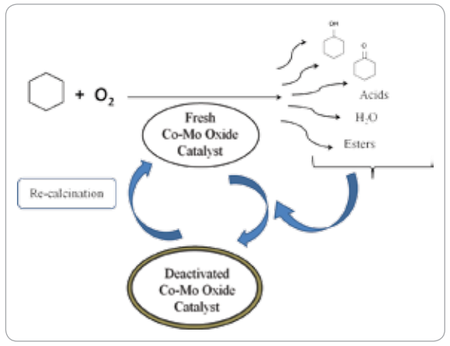
Nanofluids are suspensions of particles in the nanometer size range in conventional fluids. We have demonstrated that the mass transfer rates in such fluids is much higher (often by a factor or 2 or more) than in the base fluid alone. In ongoing work, we are attempting to (a) understand the physical basis of this effect both experimentally (through measurements of diffusivities in quiescent nanofluids) and theoretically (through multi-scale simulations), and (b) map the regions in the parametric space where substantial enhancements may be expected in industrial-type contacting equipment.

Mass transport in nanofluids

The figure shows the rate of tracer (green colour) transport is much higher into a medium containing silica nanoparticles as compared to that into a particle-less medium.

2. Catalysis of liquid phase oxidations (LPOs):

LPOs are an industrially important way to functionalize a variety of hydrocarbons and oxygen-containing compounds, but their complex chemistry and involvement of transport resistances make them difficult to study and optimize. The recent trend in this area is towards heterogenizing these reactions. A mechanistic study of various uncatalyzed and catalyzed oxidations (cyclohexane, glycerol are two examples) are being undertaken to understand the catalyst-support interaction with various catalysts, and also the reaction-engineering aspects in industrial type reactors.



We have shown Co-Mo oxides to be catalytically active and selective for cyclohexane oxidation. While product adsorption deactivates the catalyst, recalculation revives the activity.

3. A theoretical and modeling framework for solid-solid reactions

Conventionally, solid-solid reactions have been treated using models similar to solid-fluid reactions. However, in general, we need to explicitly account for the discrete nature of contact between reactants in such cases (and hence the complicated geometries that arise when reactions proceed from such contact points), since the conventional treatment often leads to inconsistent values for the rate parameter estimated (Diffusivity in most cases). We have derived approximate models to treat such situations and also derived some conditions under which the conventional treatment may suffice. In ongoing work, we are trying to rigorously solve the problem using a finite-element technique, and hence establish the regions in the parameter space where different approximations are tenable. The models are also being tested via experiments on calcia-alumina and other systems.

4. Microencapsulation in polymers and polymeric membrane synthesis:

Several gas-separation membranes and RO membranes are made by polymerization techniques in which the conditions of synthesis have a significant influence on the structure, and hence function, of the membrane. Interfacial polycondensation is a reaction that is actively being investigated in our group. Novel methods have been developed to follow the kinetics of these fast reactions and relate them to the structural features of the films that form. Other themes such as performance enhancement through particle incorporation are additional areas of interest.

An understanding of the interplay between transport and reaction kinetic factors can help unravel the structure of several seemingly disconnected applications.

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Ph. D, Indian Institute of Science, 2003

Rochish M Thaokar

Areas of Interest: Electrohydrodynamics, Biomembranes, vesicles and capsules

I have been involved in establishing an electrohydrodynamics lab to conduct experiments, theory and simulations in

a. Liquid-liquid systems, specifically Drop dielectrophoresis, electrophoresis, electro deformation and breakup (emulsification), electrocoalescence, and electrospinning, towards applications such as desalters, emulsifiers and separation units.

b. Soft matter systems, specifically charged biomembranes, spherical and cylindrical vesicles (liposomes) towards applications such as electroporation and electrofusion, elastic microcapsules for drug delivery applications and in developing an understanding of soft lithography using electric fields.

Publications:

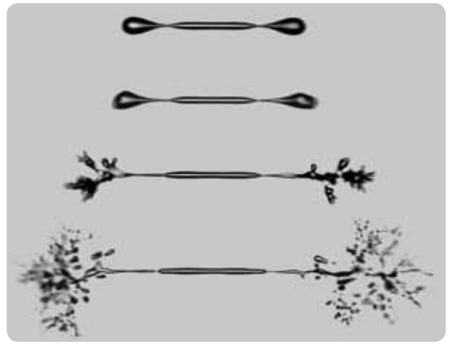
1. Karyappa, R., Deshmukh, S. and Thaokar, RM., Breakup of a conductigng drop in oil, 2014, Journal of Fluid Mechaincs (COVER PAGE),754,550

2. Sinha, P, Gadkari, S and Thaokar, RM, Electric field induced pearling in cylindrical vesicles, 2013, Soft Matter, 9, 7274-7293

3. Karyappa, R. and Thaokar, RM, Deformation and Kinetics of elastic capsules, 2014, Langmuir, 30(34), 10270

1. Drop Emulsification

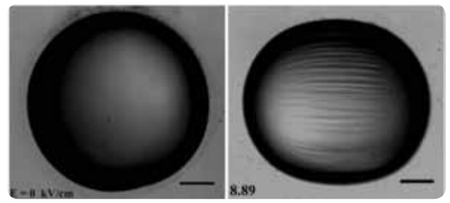
A conducting drop suspended in a viscous dielectric and subjected to a uniform DC electric field deforms to a steady-state shape when the electric stress and the capillary stress balance. Beyond a critical electric capillary number Ca, which is the ratio of the electric to the capillary stress, a drop undergoes breakup. Although the steady-state deformation is independent of the viscosity ratio λ of the drop and the medium phase, the breakup itself is dependent upon λ and Ca. We perform a detailed experimental and numerical analysis of the axisymmetric shape prior to breakup (ASPB), which explains that there are three different kinds of ASPB modes: the formation of lobes, pointed ends and non-pointed ends. The axisymmetric shapes undergo transformation into the non-axisymmetric shape at breakup (NASB) before disintegrating which are modes of charged lobes disintegration, regular jets (which can undergo a whipping instability) and open jets, respectively. We understand drop electrohydrodynamics using experiments, theory and Boundary element calculations.



Breakup of a conducting drop suspended in a dielectric fluid in a uniform electric field, (Ca, λ) = (0.4, 0.00126).

2. Electrohydrodynamics of vesicles

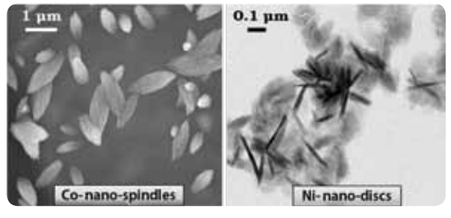
We are interested in understanding the physics of effect of electric field on vesicles. Cylindrical experiments are a good prototype for the same. Experiments show that a cylindrical vesicle when subjected to an axial electric field, displays an axisymmetric pearling instability (the Rayleigh–Plateau instability) beyond a threshold electric field. The tension required to induce the instability is produced by the electric field. At higher values of field strength however, a stabilizing action of the electric field is seen. This renders the fastest growing wavenumber, km, independent of the electric field at high electric field strength. At long times, a pearled state is observed, with the pearls separated by short cylindrical nanotubules. The focus in the group is now on understanding electroporation with applications in biomedical industry.



Wrinkling or folding instability observed on a Polysiloxane microcapsule suspended in a dielectric fluid in a uniform electric field (Scale bar = 200 μm).

3. Synthesis and characterization of elastic capsules using electric fields.

We are interested in understanding the physics of elastic capsules using electric fields. Our study indicates a new method of determining Young's modulus, Bending modulus and thickness of the membrane using electric fields. We also have a novel method of producing non-spherical capsules. We have demonstrated that electrohydrodynamics can be used to understand the mechanism of capsule formation. The aim in this study is to use electrohydrodynamics in appications of capsules in FMCG and Biomedical industry.



Hierarchical magnetic nanostructures of cobalt and nickel obtained by chemical reduction method.

The underlying theme of the lab is to harness electric fields for niche applications. The emphasis in the lab has been to improve fundamental understanding of the principles of electrohydrodynamics and interaction with interfaces with a focus on applications.

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Areas of Interest: Fluid Mechanics, Colloids & Interfaces, Biophysics

Our research focuses on fundamental problems in the area of fluid mechanics and colloids science. This covers problems in suspension flows; transport processes, film formation and cracking phenomena in drying films of colloidal dispersions; and stability of thin liquid films and sheets. In the area of colloids, we are interesed in understanding the consolidation, film formation and cracking processes in drying colloidal dispersions with application to paints and coatings, ceramics, drying and cracking of soil, and photonic metamaterials. In the area of fluid mechanics, we are interested in gaining a fundamental understanding of the atomization process aimed at relating the process conditions to the final drop size distribution. Our research work utilizes a combination of theory, computations and advanced experimental techniques such as confocal optical microscopy, electron microscopy and rheometry to name a few.

Publications:

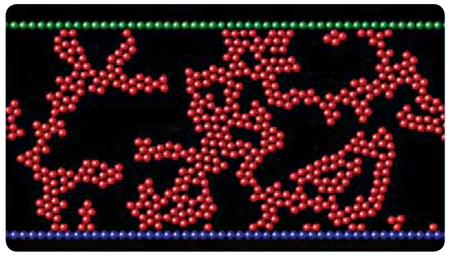
1. R. Karmakar, R. Gulvady, M. S. Tirumkudulu, and K. V. Venkatesh, “Motor characteristics determine the rheological behavior of a suspension of microswimmers”, Phys. Fluids, 26, 071905 (2014)

2. M. S. Tirumkudulu and M. Paramati, “Stability of a moving radial liquid sheet: Time-dependent equations”, Phys. Fluids, 25(10), (2013)

3. A. Sarkar, and M. S. Tirumkudulu, “Ultimate strength of a colloidal packing”, Soft Matter, 8(2), 303-306 (2012)

1. Consolidation, Film formation and Cracking Processes in Drying Colloidal Dispersions:

Our current focus in the colloids area is to engineer ordered materials from colloidal dispersions through a fundamental understanding of particle ordering and consolidation in drying colloidal dispersions with a view to direct particle assembly. Using this bottom-up approach, both structure and composition will be controlled over micro/nano length scales to achieve the desired macroscopic behavior. The study is critical to industries as diverse as electronics, paints, coatings, ceramics, and agriculture. The methodology will include an understanding of the fluid-solid phase transition for varying particle size, shape and chemistry (inter-particle interaction), followed by prediction of ordering as a function of the said parameters in the presence of external fields. Drying and consolidation processes build up stresses in the colloidal packing while packing flaws such as voids and dislocations nucleate cracks thereby compromising the mechanical integrity of such materials. The study will also focus on understanding the fracture mechanics of such materials with an aim at their prevention. The proposed research will involve developing theoretical models complemented by experiments.



The image shows a snapshot of a particle packing of colloidal particles undergoing compression. The simulations are performed using the molecular dynamics simulation code, LAMMPS.

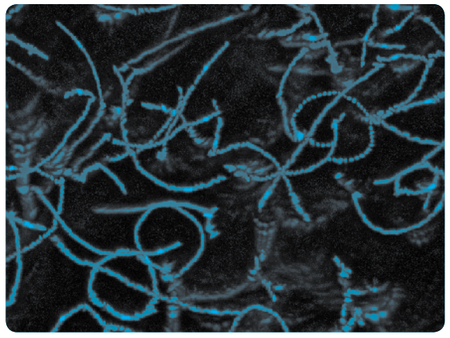
2. Atomization of Thin Liquid Sheets:

The interest here is to understand the stability of thin liquid sheets formed by impinging liquid jets, which find application in atomization processes related to combustion. We have recently shown that a radially expanding sheet is inherently unstable due to its spatially varying thickness - a fact that has been missed in the long history of its study. Our near term goal is investigate theoretically and experimentally this important aspect and predict the stability characteristics of radially expanding liquid sheets. Based on these results, we are in the process of building an atomizer for producing sub-micron droplets with minimal energy input.

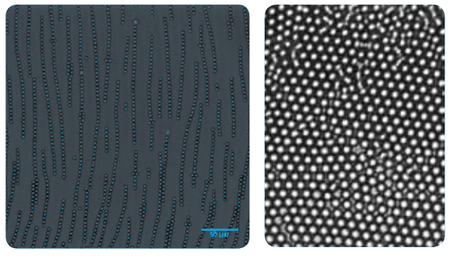
Given the current energy needs of the country, understanding the atomization process so as to control the drop size and its distribution will be critical to diverse areas such as efficient combustion of fuels in gasoline and diesel engines, spray drying and coating, and spraying for efficient dispersal of insecticides/pesticides.

3. Chemotaxis in Bacteria:

Our interest has recently been drawn to problems in biophysics where we apply the knowledge gained from studying transport processes in colloids to solve specific problems related to cell motility. As part of a collaborative project, we are studying the phenomenon of chemotaxis, which refers to the movement of microorganisms in response to chemical stimuli. This lies at the heart of understanding the mechanism of sensing and locomotion in more complex and higher organisms. While past studies have shown that unicellular prokaryotic bacteria such as Escherichia coli move up gradients of favorable chemicals via a sequence of straight swimming paths at constant swimming speeds interspersed by random turns, we have recently discovered that E. coli can also modulate its swimming speed to achieve efficient migration. This points to an unknown mechanism where in the cell is able to control its motor speed or modulate the geometry of its propellers by mere sensing of a chemical. Our immediate goal is to quantify these changes and predict the motion of bacteria in the presence of external chemical stimuli.



The image shows the track of swimming Escherichia coli using dark field microscopy. Such images provide detailed data on the swimming behavior of microorganisms such as, swimming speeds, tumble frequency, and turn angles.



Chain formation and particle ordering of colloidal particles when a colloidal dispersion is subject to electric field.

Our research focuses on fundamental problems in the area of fluid mechanics and colloids science where many of the problems are inspired by applications from the industry.

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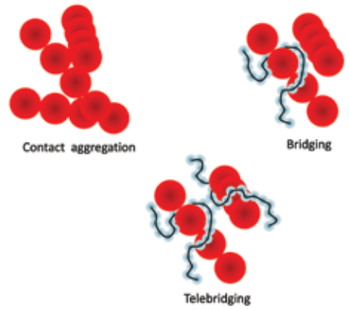
Mukta Tripathy

Areas of Interest: Soft matter systems, Polymer-nanocomposites, Self-Assembly

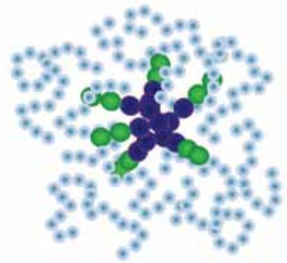
We are interested in studying the effect of anisotropies on the structure, phase behaviour, and dynamics of soft condensed matter systems. These anisotropies may be present in the elementary particles themselves, or may be emergent anisotropies on much longer length scales even while the particles themselves are purely isotropic. To that end, research in our group involves various soft matter systems of both theoretical and practical interest. These include polymer nanocomposites, Pickering emulsions, soft-penetrable particles, and surface-corrugated colloids. We use a variety of tools ranging from statistical mechanical theories to mesoscale simulations.

While our interest in polymer nanocomposites, and Pickering emulsions is of a more immediately practical nature, our interest in soft-penetrable particles and rough colloidal particles stems from an interest to understand structure and phase behavior at a more fundamental level. We work with these models to propose solutions to current problems in both theory and simulation. More recently, we have begun using statistical mechanical tools to understand biological phenomena such as how cells use intra- and extra-cellular cues to control their global gene expression profile using DNA-binding proteins.

1. Polymer nanocomposites are known to have vastly improved properties compared to pure polymer melts. Hence, the stability of these composites is of prime interest. Modern composites are made from nanoparticles such as carbon nanotubes, clay particles, and patchy particles. Our group is interested in determining the conditions where these different kinds of nanoparticles form stable dispersions with polymers. Carbon nanotube composites are of interest, particularly in the context of producing highly conducting, low-cost materials. A requirement for highly conducting nanotubes (or nanorods) to give rise to highly conducting composites is that the nanotubes/nanorods form a system-spanning percolated network. We are therefore, interested in determining the miscibility and percolation co-conditions for composites of these kinds. We also probe the complex structures formed by grafted nanoparticles in polymer melts. Our initial studies indicate that chemically anisotropic nanoparticles (such as Janus rods) as well as grafted nanoparticles are likely to form stable mesoscale structures within the melt. These materials are likely to yield interesting and tunable optical properties.



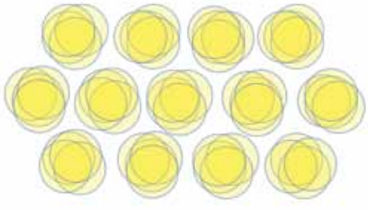
A variety of different microstructures available to nanorods as they phase separate from a polymer melt.



A colloidal micelle (made of Janus rods) within a polymer melt.

2. Soft-penetrable particles are model systems for highly coarse-grained particles used in both theory and simulations. We put forth several models of coarse-grained penetrable particles, and study their dynamics and phase behavior. Our results indicate clustering of particles that interact in a purely repulsive manner. Furthermore, at higher densities, these systems form cluster-crystals of various symmetries. When mixed with hard particles they give rise to very interesting phases. While penetrable particles are highly coarse-grained models for large and sparse molecules, surface-corrugated models for colloidal particles explicitly treat the surface roughness of real colloidal particles. We study the effect of surface roughness using various models for roughness between both charged and uncharged colloids.

3. Pickering emulsions are oil-in-water emulsions stabilized by colloidal particles (rather than surfactants). Due to their larger oil droplet size, they can be used in many novel applications (drug delivery, micro-reactors, etc.) that traditional microemulsions cannot be used for. However, most Pickering emulsions are not thermodynamically stable, resulting in short shelf-lives. From understanding gained from both soft colloidal particles and rough colloidal particles, we are interested in mapping out the narrow range of stability conditions for Pickering emulsions.



A schematic of a cluster crystal. Each lattice position in this crystal is occupied by multiple penetrable particles.

Studying soft matter is a window to understanding a wide range of physical phenomena as well as a variety of equilibrium and non-equilibrium states of matter. We are interested in making small changes at the particle level in order to understand the underlying commonalities between a large variety of emergent phenomena.

Publications:

1. Dispersion, Depletion, and Bridging of Athermal and Attractive Nanorods in Polymer Melt, Uma K, Sankar & Mukta Tripathy, Macromolecules 48, 432-442 (2015).

2. Theoretical Study of Structure and Assembly of Janus Rods, Mukta Tripathy & Kenneth S. Schweizer, Journal of Physical Chemistry B 117, 373 (2013).

3. Activated Dynamics in Dense Fluids of Attractive Nonspherical particles. I. Kinetic Crossover, Dynamic Free Energies, and the Physical Nature of Glasses and Gels, Mukta Tripathy & Kenneth S. Schweizer, Physical Review E 83, 041406 (2011)

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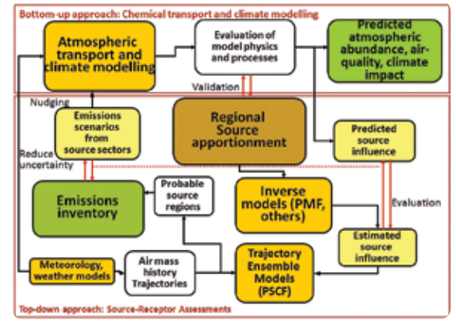
Chandra Venkataraman

Areas of Interest: Aerosol physics, chemistry and optics; simulations of air-quality and climate change; energy-emissions modelling; aerosol synthesis of nanoparticles for drug delivery

Aerosol science and engineering, the study of gaseous dispersions of micro- and nanoparticles, enables understanding of very diverse natural and engineered systems. The research in our group addresses two distinct areas of aerosol science and engineering: (i) Climate change/air quality and (ii) aerosol synthesis of nanoparticles for drug delivery. Atmospheric aerosols, or fine pollution particles, significantly change Earth's energy balance and alter cloud properties, thereby affecting climate, while also being a leading risk factor in the burden of disease from increased cardio-pulmonary and respiratory mortality. In this area, our investigations address questions like: Which economic sectors and technologies most impact climate change and air-quality? Which interventions offer the best benefits? How do aerosols modify clouds and monsoon rainfall? Aerosol synthesis of nanoparticles involves a gaseous suspension of droplets and gaseous precursors, in a flow system, wherein controlling the rates of nucleation, evaporation / surface growth and coagulation leads to control of primary particle size (and size distribution), substructure (grain boundary, pore size and crystalline state) and properties of aggregates (fractal dimension and particle bond energies). Aerosol routes allow single-step, continuous processing and direct recovery of nanoparticles as dry powders. Our research addresses the challenge of processing heat-sensitive biomaterials into therapeutic nanoparticles with controlled properties, without compromising structural integrity and activity. We study mechanisms influencing solid phase formation during drying of solution droplets to devise aerosol techniques/systems for the synthesis of nanoparticles containing drug biomolecules and genetic material.

1. Combustion particle properties and energy-emissions modelling

Emissions inventory development for research and regulatory applications, in air-quality and climate change, needs explicit linkages to emitting technologies and to the microphysical, chemical and optical properties of emitted particles. The influence of residential solid fuel use on climate over India, through substantial emissions of black carbon particles was first described through work from our laboratory (Venkataraman et al. 2005, Science, 307(5714), 1424-1426). Ongoing research addresses understanding emission aerosol from dispersed tradition combustion sources (residential biomass stoves and kerosene lamps, brick kilns, agricultural field burning) and multi-criteria mitigation analysis to provide decision and policy support.



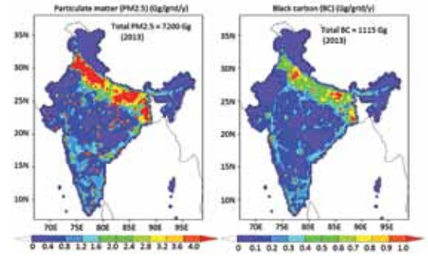
Top-down and bottom-up approaches to reduce uncertainties in regional air-quality and climate simulations.

2. Simulations of aerosol-induced changes in the radiation balance, clouds and precipitation over India

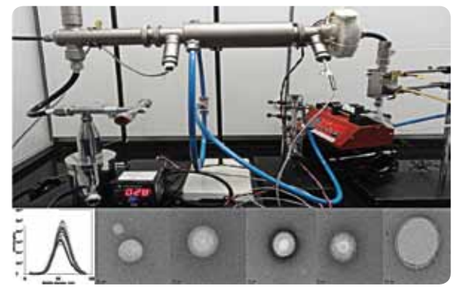
Understanding the physics of aerosol-mediated atmospheric processes, which influence rainfall is imperative to India's rain-fed agricultural economy. Mechanisms of alteration of clouds and rainfall by aerosols are being studied through simulations using climate models (ECHAM-HAM, WRF-CMAQ/CAMx) and statistical approaches applied to satellite derived cloud and climate variables. This work seeks to improve the physics of climate models to better predict regional climate change.

3. Aerosol synthesis of nanoparticles with controlled properties for drug delivery applications

Therapeutic nanoparticles with controlled properties enable control over therapeutic outcomes, through drug targeting to specific sites, enhancing cellular uptake, protection against drug inactivation and achieving controlled drug release. A pulse-heat aerosol reactor has been designed and built to prepare lipid nanoparticles with controlled size, morphology, crystallinity and controlled release properties. Experimental studies investigate nanoparticle surface modification, layered nanoparticles and the encapsulation of drug molecules and genetic material, while modelling studies address mechanisms governing control of nanoparticle properties during droplet drying, to engineer nanoparticles for new applications.



Spatial distributions of annual emissions of particulate matter ($PM_{2.5}$) and black carbon (BC) from Indian industrial, transport and residential energy-use.



Pulse heat aerosol reactor and synthesized lipid nanoparticle mobility size distributions and microstructure (TEM images).

Our methodologies combine fundamental experimental studies with multi-scale modelling to better understand aerosol processes in engineered and natural systems. We devise systems and solutions, for application in fields as diverse as climate change, air-quality and drug delivery.

Publications:

1. Venkataraman, C. and Pawar, A. A. (2015), Method and a system for producing thermolabile nanoparticles with controlled properties and nanoparticles matrices made thereby, Divisional US Patent Application No. 14/644,463, Filed on Mar-11-2015.
URL: https://www.google.co.in/patents/US20130035279

2. Sadavarte, P. and C. Venkataraman (2014) Trends in multi-pollutant emissions from a technology-linked inventory for India: I. Industry and transport sectors, Atmospheric Environment, 99, 353-364, doi:10.1016/j.atmosenv.2014.09.081

3. Cherian, R., C. Venkataraman, J. Quaas, and S. Ramachandran (2013), GCM simulations of anthropogenic aerosol-induced changes in extinction, atmospheric heating and precipitation over India, Journal of Geophysical Research-Atmospheres, 118, 2938-2955, doi:10.1002/jgrd.50298.

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K V Venkatesh

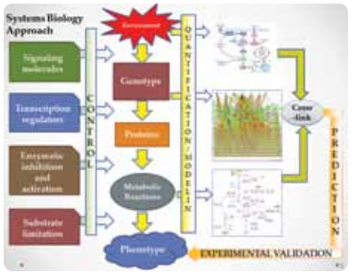
Areas of Interest: Bio-Systems Engineering: Systems and Synthetic Biology, Metabolic Engineering, Modeling of Metabolic Diseases, Network Analysis of Gene Regulatory, Signaling and Metabolic networks

Biological systems are highly interconnected and hierarchical with unique structures, which are being discovered by molecular biologists. Our group is interested in developing novel computational and theoretical methods to analyze biological structures to link genotype to phenotype. Our main focus has been in interfacing engineering principles with biology and medicine. We have applied engineering design principles to biological systems to obtain insights into its evolution, operation and regulation by developing novel theoretical methodologies to analyze biological networks at genetic, signaling and metabolic levels. The design principles inherent in living systems have been experimentally demonstrated in our lab. Our group was one of the first to reverse engineer the design prevailing in a microorganism to a physical system thus demonstrating the relevance of using engineering principles in both living and non-living systems.

Quantification of biological processes help us organize seemingly disparate subsystems into a coherent whole, discover new strategies for controlling them, compute their limits, understand underlying mechanisms and add to or correct existing knowledge of their behavior.

1. Understanding Bacterial Metabolism

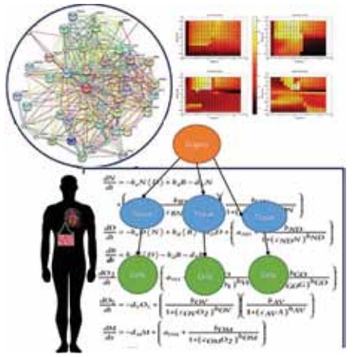
Escherichia coli is a facultative anaerobic bacterium capable of surviving with (aerobic) or without (anaerobic) oxygen. We study the effect of key transcriptional regulators on the growth of E. coli under different aeration conditions. The substrate intake is directed towards three main objectives, namely, energy balance (ATP synthesis and consumption), biomass synthesis (growth and biopolymer synthesis) and redox balance (NADH synthesis and consumption). Our focus is to answer the relevant question as to whether *the global transcriptional regulators have a role in optimizing growth to achieve the three objectives and if so what is the exact mechanism of their control?*



Genotype to phenotype - a comprehensive study of metabolism to understand the underlying molecular mechanisms by genomic scale modelling and linking of signalling, gene regulatory and metabolic pathways along with experimental validation.

2. Whole body Metabolic Models in Humans to Study Metabolic Diseases

Characterizing disease in mammalian systems is challenging due to the inherent complexity in the system. Diseases such as cancer are found to be multi-factorial and nonlinear Systems biology techniques enable us to model disease conditions using a holistic approach. The disease condition is an emergent property arising from defects in signaling, genetic and metabolic levels rather than defects in individual biological entities. The main questions we try to answer are – *(i) what parameter or sets of parameters shift the physiological state of a human from healthy to diseased state? (ii) How sensitive are these parameters to perturbations? (iii) Can the parameters be controlled? If so, how effective is it?* To address these, we have developed a comprehensive whole body metabolic model incorporating several organ types and signaling networks.

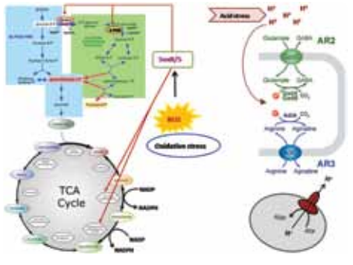


Dynamic modelling of the whole body metabolism in humans and network analysis.

3. Network Analysis in Biological Systems

We have performed genetic, signaling and metabolic network analysis for various biological systems.

- Genetic networks: Tryptophan Regulation and Steady state analysis of gene regulatory network in E. coli, Mathematical models of GAL regulon in yeast in conjunction with guided experiments have demonstrated system-level properties such as ultrasensitivity, memory, noise attenuation, rapid response, and sensitive response arising out of molecular interactions.
- Signaling Networks: Analysis of Osmoregulation in yeast; G-protein mediated calcium oscillations; Quantification of chemotaxis in E. coli to varying concentration and gradients; Simulation of switch-like PIP3 response using a two-compartment computational model in chemotaxis of immune cells, Modeling of spatially localized G-PCR signaling to execute polarized cell response;
- Metabolic Networks: Phenotypic state analysis in C. glutamicum; Hyperosmotic state in S. cerivisae; Metabolic flux analysis of E. coli; Phenotypic analysis of L. rhamnosus during growth on mixed substrates.



Genomic scale modelling and experimentation to understand the molecular mechanisms underlying multiple stress resistance in bacteria.

Publications:

1. Optical Control Demonstrates Switch-Like PIP3 Dynamics Underlying The Initiation Of Immune Cell Migration. W.K.A. Karunarathne, L. Giri, A.K. Patel, K.V. Venkatesh, and N. Gautam, Proceedings of National Academy of Sciences 2013 110 (17) E1575-E1583.

2. P.R. Somvanshi and K.V. Venkatesh, "A conceptual review on systems biology in health and disease: From Biological networks to potential therapeutics" Perspectives in systems biology, Systems and Synthetic Biology Journal, Springer. Aug 2013.

3. Steady state analysis of the genetic regulatory network incorporating underlying molecular mechanisms for anaerobic metabolism in Escherichia coli, S. Srinivasan, K.V. Venkatesh, Molecular BioSystems, 2014.

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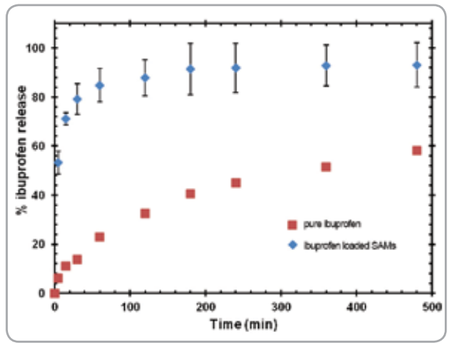
Areas of Interest: Drug delivery, aerogels, supercritical carbon dioxide, micronization

Many available drugs and those being discovered are poorly soluble in water. Reducing their size and/or loading them in drug delivery vehicles improve their bioavailability. My research focuses on several processes to reduce the size of drugs by using sub- and supercritical carbon dioxide. In my laboratory, aerogels are used as drug delivery platforms. Aerogels are light particles with high surface area, pore volume and porosity suitable for drug delivery. Developing inexpensive processes for preparation of aerogels from biocompatible sources for high drug loading and their controlled release forms the central aim of research on aerogels. Experiments and modeling of the processes are carried out to understand the micronization and the aerogel processes.

1. Project 1:

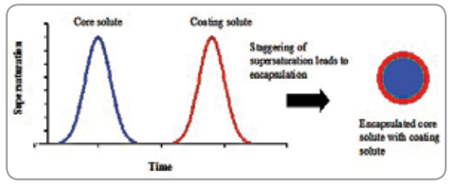
An improved process for preparation of silica aerogel microparticles (SAMs) for drug delivery from rice husk ash (RHA), an inexpensive source rich in biocompatible silica, has been developed. The wet gel microparticles were produced by a sol–gel method using water-in-oil emulsion, where a mineral oil replaced vegetable oil for easy separation using less energy. Taguchi design of experiments was used to optimize the parameters controlling the sol–gel method. The wet gel particles were dried with supercritical carbon dioxide ($scCO_2$) to obtain SAMs. They were characterized by their properties such as BET surface area, pore volume, pore diameter and morphology. The efficacy of the improved process was validated by loading a water insoluble drug, ibuprofen, and a food preservative, eugenol, in SAMs from $scCO_2$ medium. SAMs had a total porosity of 99.34%, surface area of 652 m^2/g and a pore volume of 3 cm^3/g. High loadings of 0.87 g ibuprofen/g of aerogel and 8.1 g eugenol/g of aerogel were obtained. Nearly 80% of the ibuprofen was released in 30 min from SAMs compared to 14% of ibuprofen sold in the market. High loading and fast release kinetics confirmed that SAMs produced by the process are suitable for drug delivery.



Release profiles of ibuprofen loaded in silica aerogels ◆ and crystalline aerogels ■

2. Project 2:

A rapid pressure reduction over a CO_2-expanded organic solution, from 30–70 bar to 1 bar, decreases the solution temperature by 30–80 K in a short span of time (0.5–1.5 min). This decrease generates a rapid, high, and uniform supersaturation of the dissolved solute in the solution and facilitates its precipitation as ultrafine particles. A model is developed to estimate the supersaturation, nucleation and growth rates during the pressure reduction and the particle size distribution of the precipitated particles. Cholesterol has been chosen as a model solute and acetone as a solvent. Equilibrium solubility of solute is affected by CO_2 mole fraction and solution temperature during pressure reduction. Size distributions of the precipitated particles have been calculated assuming primary nucleation (homogeneous and heterogeneous nucleation) and diffusion-limited growth kinetics. The particle sizes predicted by heterogeneous nucleation are found to be closer to the measured sizes than homogeneous nucleation.



Mechanism for encapsulation of core solute with coating solute

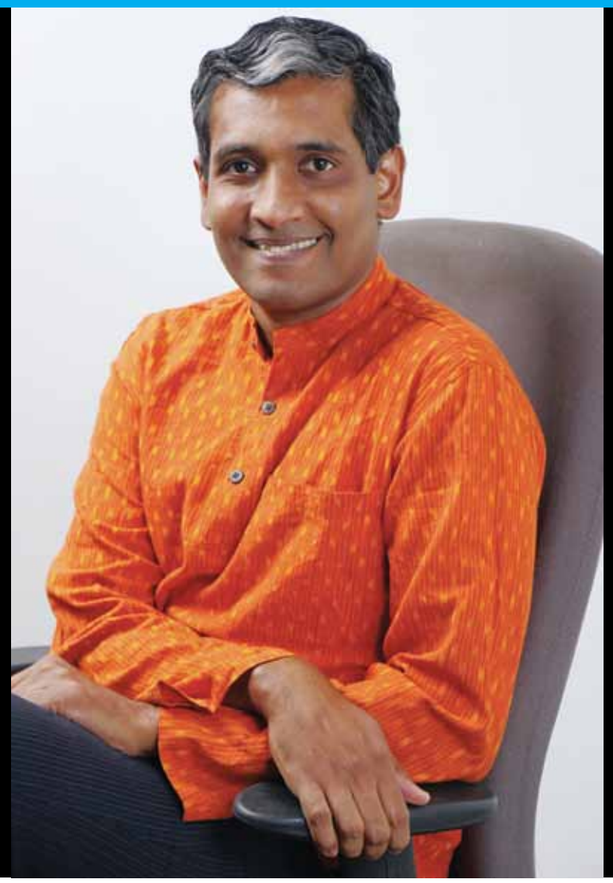
Publications:

1. Kumar, S.R., Vinjamur, M., Mukhopadhyay, M., Silica aerogels from rice husk ash for drug delivery, In Press, Industrial Engineering and Chemistry Research.

2. K. Arjun Kumar, Rajarshi Chattaraj, Umesh Dhumal, Mamata Mukhopadhyay, Madhu Vinjamur, Sameer V. Dalvi, Modeling of Precipitation of Ultra-fine Particles by Pressure Reduction over CO_2-Expanded Liquids, The Journal of Supercritical Fluids, 79, 227-235, 2013.

3. M. Vinjamur, M. Javed and M. Mukhopadhyay, Encapsulation of nanoparticles using CO_2-expanded liquids, The Journal of Supercritical Fluids, 79, 216-226, 2013.

Aerogels made from rice husk ash that contains biogenic silica offer » 99% porosity, » 650 m^2/g surface area and loading of » 0.85 g ibuprofen/g of aerogel. They are promising vehicles for delivery of hydrophobic drugs.



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Areas of Interest: Systems biology, Signal transduction, Stochastic dynamics, Reactor engineering

Dr. Viswanathan's group is currently conducting research in quantitative analysis of Tumor Necrosis Factor alpha (TNFα) signaling. The main objective of the lab is to identify, using a combination of system biology based experimentation and mathematical modeling, the mechanism that governs the phenotypic response exhibited by cells exposed to cytokine TNFα. The emphasis is on finding reliable, predictable strategies for modulation of cellular response to TNFα stimulation.

The lab is also involved in construction, and topological and dynamical analyses of biological – signal transduction, regulatory and metabolic – networks. The group is using nonlinear dynamics to characterize pattern formation in packed-bed reactors.

Publications:

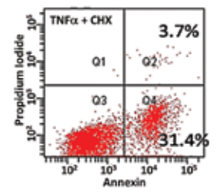
1. Dhananjaneyulu V, Sagar VNP, Kumar G, Viswanathan GA. Noise propagation in two-step series MAPK cascade. PLoS One. 2012;7:e35958.

2. Krishnakumar S, Durai DA, Wangikar PP, Viswanathan GA. SHARP: Genome-scale identification of gene-protein-reaction associations in cyanobacteria. Photosynthesis Research. 2013;118:181-190.

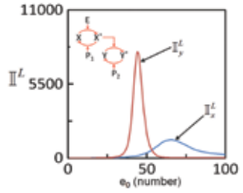
3. Narendiran K, Viswanathan GA. Impact of Wall Heat Transport on Formation of Transversal Hot Zones in Shallow, Non-adiabatic Packed-Bed Reactors. Ind. Eng. Chem. Res. 2015;54:7352–7363.

1. Systems biology of Tumor necrosis factor alpha (TNFα) signaling

TNFα, a pleiotroiphic cytokine can trigger both pro-apoptotic and pro-survival responses. It has been implicated in cancer treatment, inflammation and autoimmune diseases. The main goal is to perform systems biology mathematical modeling based single-cell experimentation to identify the key molecular signatures of the TNFα signaling network that govern the phenotypic response of a cell exposed to the cytokine. Specifically, the focus is in identifying the optimal set of proteins alteration of whose normal functioning would cause the cell to achieve specific, predictable phenotypic response following exposure to TNFα. TNFα network contains many topological substructures such as interlinked feedback loops which affect the specific phenotype expressed. The lab is interested in understanding the purpose of these substructures and the role it may play in governing the eventual phenotype exhibited by the cell.



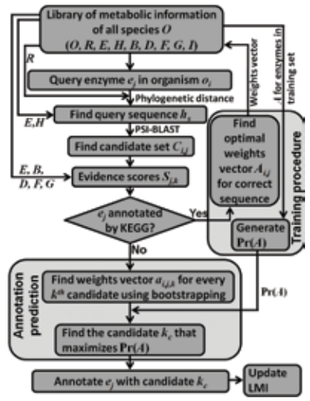
Jurkat T-cells undergoing apoptosis following exposure to TNFα and Cycloheximide (CHX). Apoptosis detection via Annexin V staining in a population of cells achieved using flow cytometry.



Intrinsic noise propagates during signal transduction through series enzymatic cascade consisting of two sequential phosphorylation-dephosphorylation cycles. Noise is amplified for a certain range of total number of upstream enzyme e_0. Noise estimated from 5000 trajectories simulated using Gillespie algorithm.

2. Construction and analysis of signaling, metabolic and regulatory networks

Manual and automated curation approaches are used to develop novel, efficient, systematic methods for construction of signaling, regulatory and metabolic networks. The group is presently involved in developing well-annotated, comprehensive mammalian TNFα signaling network and in identifying the sub-structures and modules that would govern the overall functioning of the network. Recently, the lab has initiated work towards construction and analyses of regulatory and metabolic network of cyanobacteria with a view to develop strategies for engineering the strains for production of biofuel precursors.



Flow chart depicting the methodology of "Systematic, Homology-based Automated Re-annotation of Prokaryotes (SHARP)" that uses distant-context based sequence similarity, functional region similarities, bidirectional hits for gene-protein-reaction (GPR) association prediction. 3781 new GPR associations in 10 different bacterial species predicted using SHARP led to filling 7718 gaps in the metabolic network.

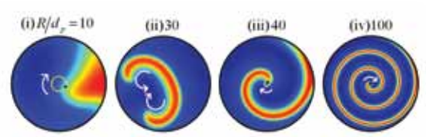
3. Noise propagation in signaling networks

Cells are constantly exposed to inevitable fluctuations or noise from variety of sources. These fluctuations propagate along with the signal and may strongly affect the phenotypic response exhibited by the cells. The lab is interested in characterizing noise propagation in various conserved modules of mammalian signaling networks such as the enzymatic cascades.

4. Pattern formation in catalytic packed-bed reactors

Catalytic packed-bed reactors are workhorse of chemical, petrochemical and pharmaceutical industries. The focus is tp predict the formation of spatiotemporal patterns in non-adiabatic catalytic, packed-bed reactors (PBRs) with an objective to identify the parameter range for safe operation of the reactor. Nonlinear dynamics of the patterns formed in PBRs are characterized using singularity theory and numerical bifurcation analyses.

Enzymatic cascades activated during TNFα signaling can simultaneously act as signal amplifier and guarantee signal fidelity, and may also facilitate modulation of both pro-apoptotic and pro-survival responses.



Transversal spatiotemporal temperature pattern formation during ethylene hydrogenation in catalytic packed-bed reactors. Increase in reactor diameter causes a transition from rotating patterns (at $R/d_p = 10$) to spiral patterns (at $R/d_p = 40$). d_p is the catalyst particle diameter.

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Ph.D, University of Iowa, 1995

Pramod P Wangikar

Areas of Interest: Algal biofuel, metabolic engineering, enzyme engineering, biotransformation

We are primarily interested in (a) Enzyme Engineering for chiral synthesis and (b) Metabolic Engineering and bioprocess development for algal CO_2 capture and utilization (CCU). With enzyme engineering, we will deliver cost effective and environmentally friendly technology for chiral synthesis of drug intermediates. We have been working on microbial oxidoreductases, a class of enzymes with potential in chiral synthesis of commercially important secondary alcohols. High cost of the enzymes, recycling of enzymes and cofactors are some of the challenges in the field. Algal CCU on the other hand has impact in two distinct domains; (i) capture and utilization of CO_2 from stationary emitters such as power plants, steel or cement plants or refineries and (ii) a renewable source of fuel and products that are typically derived from petroleum. We work with local strains of algae that grow well under local climatic conditions of sunlight, temperature and are tolerant to high CO_2 levels. Metabolic engineering efforts are in the direction of designing strains for photoautotrophic production of usable biofuel while process development begins with detailed physiological characterization of strains under laboratory as well as outdoor conditions. We work closely with industry partners and academic collaborators on all our projects.

1. Enzyme Engineering for Biotransformation:

Deployment of enzymes in industrial production of chemicals requires development on three fronts: (i) Design of enzymes with desired characteristics of activity, selectivity, stability, substrate tolerance, etc., (ii) Cost effective production of the enzyme and (iii) Development of biotransformation process. Wangikar lab's current efforts are on all three fronts with focus on developing processes for chiral synthesis using two classes of enzymes; nitrilase and alcohol dehydrogenase (ADH). Design of enzymes is initiated with experimental testing of unexplored sequences of putative enzymes followed by directed evolution of promising candidates. We also undertake rational, model based design of enzymes in collaboration with other groups that have expertise in protein X-ray crystallography. Currently, the group has designed novel ADH enzymes that show >99% stereoselectivity and > 100 units activity / ml of fermentation broth. We envisage the use of whole cell biocatalyst for cost effective chiral synthesis. We have also designed a cofactor recycle system with a recycle ratio of 1:2,000.

B. Algal CO_2 capture and utilization (CCU):

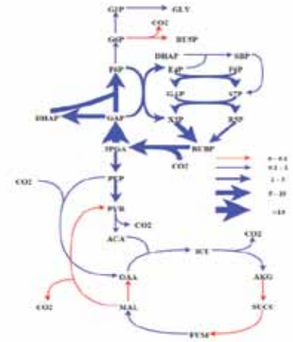
Atmospheric CO_2 levels have been rising at alarming rates over the last two centuries, and are projected to reach 700-1000 ppm (parts per million) by year 2100. Carbon and energy accounting reveals that a typical microalgal CCU is far from being net carbon negative or net energy positive, primarily because of high operational energy requirements. Further, even a medium sized Thermal Power Station would require algal ponds of over hundred square kilometers, thereby posing the challenge of capital and scale. Wangikar's group works towards design of algal strains and processes to improve the aerial productivity. Their strain selection criteria include: (i) volumetric and aerial productivity, (ii) biomass concentration at the end of batch, (iii) tolerance to local climatic conditions, (iv) tolerance to CO_2 and other flue gas components, and (v) ability to synthesize storage molecules. Algal strains isolated from the plant site of our industry partner fulfill many of these requirements and are now ready to be tested for CO_2 capture at the plant site. Apart from this, Wangikar's group also works on metabolic engineering of cyanobacteria for photoautotrophic production of high value compounds. This includes physiological characterization, genome sequencing, metabolic model construction, flux analysis and several other systems biology approaches. We have performed 13C flux analysis on model strains of cyanobacteria with current efforts on local strains. Further, we have identified a number of cyanobacterial promoters that are under the control of an internal circadian clock.

Publications:

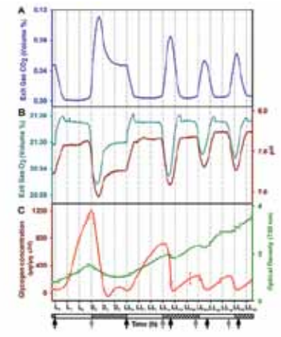
1. Gaudana, et al., Rhythmic and sustained oscillations in metabolism and gene expression of Cyanothece sp. ATCC 51142 under constant light, Front. Microbiol, 2013.

2. Alagesan, et al., Metabolic flux analysis of Cyanothece sp. ATCC 51142 under mixotrophic conditions. Photosynthesis Res, 2013

3. Sohoni et al, Optimization of high cell density fermentation process for recombinant nitrilase production in E. coli, Bioresource Technol. 2015



^{13}C Metabolic flux analysis of cyanobacteria. Our results show relatively low flux through the TCA cycle compared to Calvin cycle. Further, the photorespiration flux is negligible making this an efficient chassis for metabolic engineering. The flux values were obtained using dynamic labeling data of 17 metabolites.



Metabolic oscillations in cyanobacteria. Profiles of (A) CO_2 and (B) O_2 in the exit gas (cyan), pH of the growth medium (brown), (C) intracellular glycogen (red) content and growth (green) in the fourth day of entrainment under alternating light/dark cycles (LD) followed by constant light (LL). The horizontal bar below the X-axis denotes the light (clear), dark (shaded) and subjective dark (shaded with slanted lines) phases.

We use tools of bioinformatics, systems biology, molecular modeling and molecular biology in combination with bioprocess development to design enzymes and micro-organisms for potential applications in industrial processes. Current focus is on chiral synthesis and photoautotrophic organisms for bioenergy.

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K P Madhavan

Areas of Interest:
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2. Model Based Linear and Nonlinear Control
3. Process Optimization
4. Process Systems Engineering

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Areas of Interest:
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Areas of Interest:
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Areas of Interest:
1. Basic and detailed engineering design of process and utility systems
2. Process equipment design
3. Energy systems
4. Process safety and project execution
5. Rotating machinery

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2. Radiation Physics
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MS, University of Massachusetts, 1975

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2. Process equipment design
3. Energy systems
4. Process safety and project execution

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Support Staff

Extension and Outreach Activities

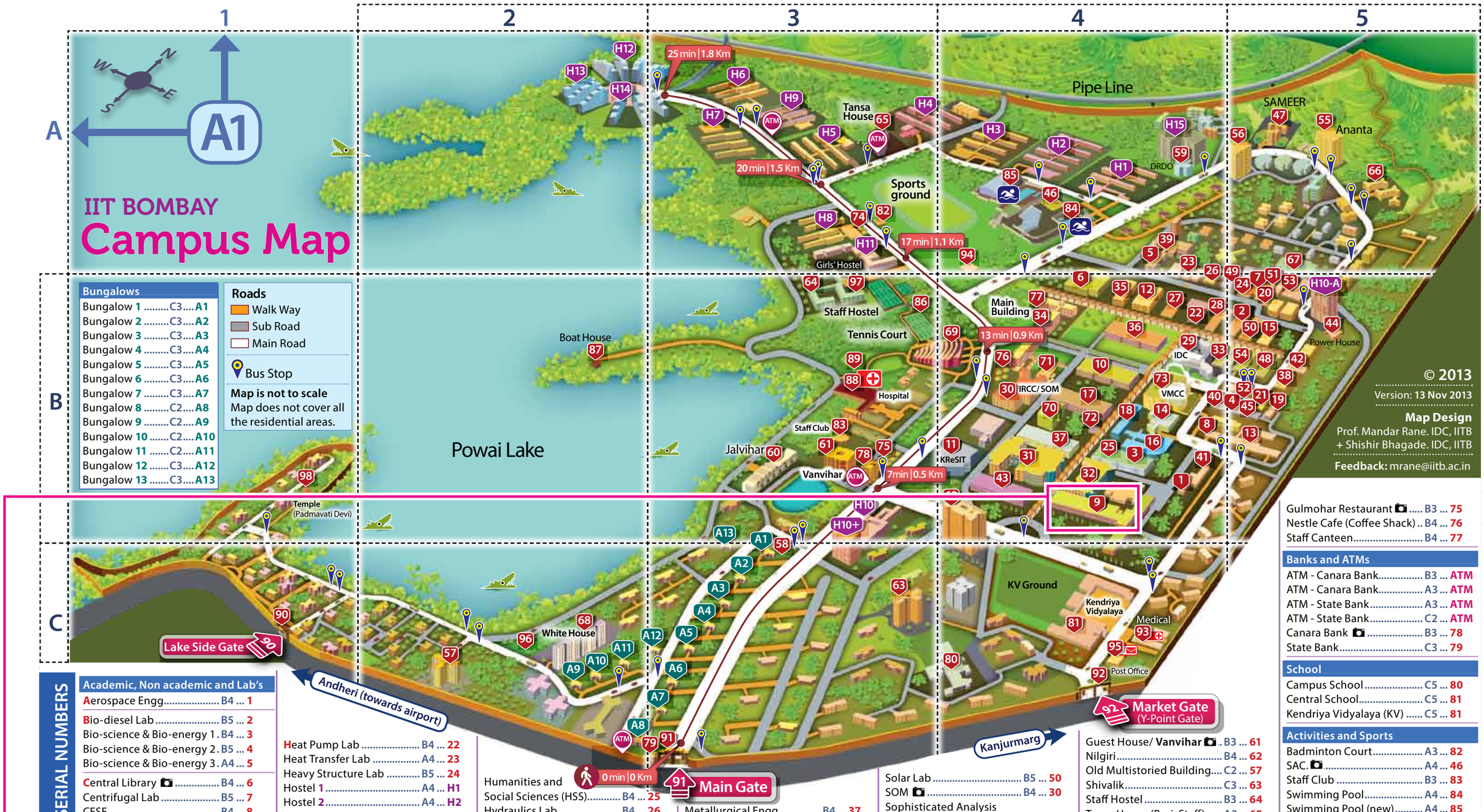
The Department actively engages with industry and other research organizations through short term courses under the Continuing Education Programme (CEP). Faculty of the department offer diverse courses in both basic and specialized areas of chemical engineering. In the last five years, 57 courses were offered of which 34 courses were specialized to suit the needs of specific organizations and run as in-house courses, while the remaining were offered as open courses at IIT Bombay. Some of the courses offered under CEP are

1. Online piping engineering course
2. Distillation and process control
3. Elements of chemical engineering
4. Introduction to systems and synthetic biology
5. Reaction Engineering
6. Piping Engineering
7. Metabolic Engineering
8. Chemical process risk analysis and management
9. Advanced materials and delivery devices
10. Multivariate statistics for process data analysis
11. Solid handling processes
12. Process simulations in industry
13. Teaching methods in engineering programmes
14. LOPA and Bow- Tie analysis
15. Bioinformatics
16. Improving process safety through hazard evaluation
17. Computing techniques for solving engineering problems
18. Underground coal gasification- theory and practices
19. Digital Control from Scratch
20. Open Source Tools Hands-on Course on Arduino Microcontroller, PLC, and Sandhi, a LabVIEW alternative

The faculty of the department have also developed courses under the National Programme on Technology for Enhanced Learning (NPTEL). A total of 11 courses have been offered under the NPTEL of which 6 courses were web-based and the remaining were video recorded. Some of these courses include Process Control, Fundamentals of Heat and Mass Transfer, State Estimation and Biochemical Engineering.

Student Life

Students at IITB experience a rich life outside academics. The hostel life at IITB is legendary with friends made and experiences remembered for life. The campus is situated in a green hub of the city, surrounded by lakes, and offers a serene atmosphere to nurture both academics and extra-curricular activities. At the institute level, international cultural events such as MoodI and technical events such as TechFest are well known and keenly attended every year. At the department level, the Chemical Engineering Association (ChEA) organizes Research Scholar Symposium (RSS) to highlight the post-graduate research. ChEA organises AZeotropy, an undergraduate technical meet, with competitions and lectures related to topics in chemical engineering.



Bungalows

Bungalow 1	C3	A1
Bungalow 2	C3	A2
Bungalow 3	C3	A3
Bungalow 4	C3	A4
Bungalow 5	C3	A5
Bungalow 6	C3	A6
Bungalow 7	C3	A7
Bungalow 8	C2	A8
Bungalow 9	C2	A9
Bungalow 10	C2	A10
Bungalow 11	C2	A11
Bungalow 12	C3	A12
Bungalow 13	C3	A13

Roads
- Walk Way
- Sub Road
- Main Road

Bus Stop

Map is not to scale
Map does not cover all the residential areas.

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Version: 13 Nov 2013

Map Design
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+ Shishir Bhagade. IDC, IITB

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SEARCH BY GROUPS AND SERIAL NUMBERS

Academic, Non academic and Lab's

Residential

Auditoriums and Halls

Food

Banks and ATMs

School

Activities and Sports

Others and Medical

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Design:
Nirmal Biswas (Picatype Design Studio)

Photograpy:
Devendra Parab

Printed and Bound by:
New Jack Printing Press Pvt. Ltd.

Printed in India
First Edition (2016)

Disclaimer: The editorial content, views and opinions expressed in this book are from Individual contributors and not necessarily those of Department of Chemical Engineering, IIT Bombay, the publisher and or editors.

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