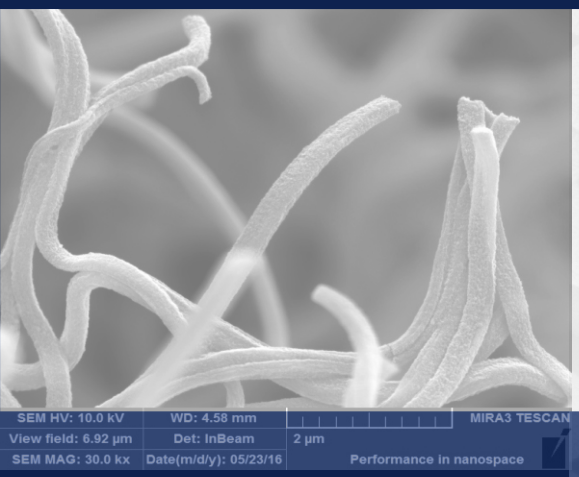
Department of Chemical Engineering

Indian Institute of Technology Kanpur



Picture Courtesy: Dr. Rahul Mangal

https://www.iitk.ac.in/che

Contents

Message from Department Head

Welcome to the Department of Chemical Engineering at IIT Kanpur. The department is ranked among the nation's top schools in chemical engineering and has been built over the years by faculty members, who have always been exceptionally hard-working, highly dedicated to research and committed to provide cutting edge knowledge and rigorous training to our students. Our core mission is to fully prepare our engineering graduates to be leaders of industry and society. Developing their advanced technical and problem-solving skills, ability to effectively and persuasively communicate and develop an understanding of how to best serve the society are our focus. Our undergraduate and graduate programs provide the unique interdisciplinary academic foundation and scholarly training needed to address complex engineering problems. We carry out research in core areas of chemical engineering such as fluid mechanics, thermodynamics, separation processes and controls as well as interdisciplinary areas such as nano sciences and technology, biosciences, soft matter physics, advanced materials and high-performance computing.

Over the next few years, the department is also launching exciting new initiatives to improve the technical skills of our students and opportunities to use those skills to solve real life problems facing our society. We have made plans to leverage powerful machine learning and data science tools to train our students in advanced computational skills that will give them a competitive edge since we now recognize data science will significantly enhance our capacity to do advanced engineering and we are committed to being positioned at the forefront of that revolution.

We provide a vibrant learning and working environment. We foster a sense of collective efficacy among our faculty and share the belief that, together, we can make a difference in the lives of our students and society. We maintain an atmosphere of diversity, equity and inclusion, academic integrity, and respect as a way of life.

We take great pride in our alums, amongst whom we have recipients of almost all significant national and international recognitions: National Science Medal by the President of the United States of America, Membership of the National Academy of Science (USA), National Academy of Engineering (USA), National Medal of Technology and Innovation (USA), Infosys prize, Shanti Swaroop Bhatnagar prize, TWAS prize and many more.

Through this brochure, we provide you a glimpse of what we are today in the hope that it will stir your curiosity enough to consider ChE@IITK as a destination for meaningful academic pursuits. Feel free to drop us an email for any further queries or to drop by for a tete-a-tete over a cup of tea. Thank you for your interest.

Prof. Jayant K. Singh
Head, Department of Chemical Engineering

Department at a Glance

Department of Chemical Engineering is among the five departments established at the inception of IIT Kanpur in 1959. Along with other pioneer departments, it ushered in a new paradigm in undergraduate engineering education that fosters the creative thinking process in a very open and vibrant academic environment. From an early emphasis on developing and perfecting the undergraduate curriculum to nurturing a fledgling post-graduate research program to significantly contributing to applied and fundamental ChE research, we have grown from strength-to-strength over the past several decades.

Ranked among the nation's top schools in Chemical Engineering, the department at IIT Kanpur is now endowed with state-of-art facilities and distinguished faculty members with both national and international recognitions. The 25 current faculty members with expertise in traditional as well as emerging areas of chemical engineering are at the forefront of nurturing the vibrant academic ambience of the department through their research and pedagogical endeavours. They are ably supported by 20 technical and secretarial staff members. The department has also hired several postdoctoral fellows, as a part of an Institute-wide initiative for supporting research activities. Several of our faculty members are Fellows of all the Indian Academies of Sciences and Engineering, and many serve on the editorial boards of national and international journals. They have also been recognized by prestigious awards such as the Infosys Prize, Shanti Swarup Bhatnagar Prize, Herdillia and Amar Dye Chem awards of the Indian Institute of Chemical Engineers.

A hallmark of our department is the emphasis on quality education as reflected in the over 50 “labor of love” textbooks written by our faculty, many receiving international acceptance. This is complemented by a strong research ethos, carefully nurtured by the pioneers and effectively passed on from one generation to the next. The significant research funding has brought in a critical mass of young, talented and motivated faculty immersed in research in the frontier areas of complex fluids, micro-reactors, nano-technology, adhesion, molecular simulation, biocomputation. This is in addition to research in tradition areas of fluid dynamics, conventional/new separation processes, catalysis, polymer engineering and process design and control.

Over the past two decades, in line with global trends, high-impact research has naturally witnessed a greater emphasis on PG programs, particularly the PhD program, where students research a problem in depth. Accordingly, the PhD program has substantially expanded in size with ~100 PhD scholars currently working on challenging and contemporary research problems. In parallel, the department's publication profile too has witnessed a quantum leap, both in terms of quantity and quality, with articles making it to the top-most scientific journals. The rigour of the PhD program is reflected in these graduates being eagerly sought by other IITs and NITs for faculty positions. Approximately 51% (i.e. about half) of the PhD graduates in the period 2015-2022 are now faculty members in Centrally Funded Technical Institutes (CFTIs). Many of them are being recognized for excelling in their chosen research areas. The BTech program of the department has historically attracted exceptional students, and continues to do so. The UG course structure at IITK is unique and flexible and our focus is definitely inclined towards responding to market forces. Keeping that in mind, we have introduced courses such as Data Science and Chemical Engineering and emphasized on experiential learning, and early exposure to computation and hands-on experiments. The department's two year MTech

program has traditionally attracted outstanding students from across the country. Our UG and PG students are encouraged to chart their own path, be it academia, industry or incubation of companies. They continue to be employed by organizations like ITC, Unilever, Shell, GE, Dow Chemicals, Dr. Reddy's Lab, Michelin, etc. Several others join core chemical engineering companies like HPCL, ONGC, IOC, GAIL, Lurgi, L&T, etc. and some of our graduates are also placed as civil servants in federal organizations.

The department's faculty members and their research groups have traditionally placed great emphasis on disseminating their research carried out in the department through peer reviewed international journal publications. As per the ISI Web of Science, the department publishes about 90+ papers per year in peer reviewed journals (4-5 publications per faculty per year), and many of the publications appear in international journals of repute.

Apart from peer reviewed journal publications, our faculty members are active in developing technologies and filing patents. Our students and faculty are constantly exploring the possibility of commercializing their inventions so that technologies developed can be of substantial benefit to the society. Some of the technologies have been transferred to company or led to the incubation of companies. Faculty members are actively involved in start-ups based on the research and development in their labs. E-Spin Nanotech Private Limited company, which designed and developed SWASA N95 mask, is a well-known example. In addition, a substantial fraction of our faculty members are involved in industrial research and consultancy. The departmental also receives external funding (from both governmental and industrial organizations) on the average of about 5 crores per year, over the last few years.

Over the years, we have made significant research contribution in core areas of chemical engineering such as transport phenomena, thermodynamics, kinetics, process engineering, catalysis, optimization and control and separation processes to areas related to advanced materials, complex fluids and soft interfaces, energy and environment and nano-sciences. With the discovery of several novel phenomena and innovative ideas, we have not only published in top international journals but also have collaborated with range of industries in addressing fundamental scientific problems with great potential practical significance. Through previous research grants we have significantly diversified and improved facilities and expertise in our department. Our Post Graduate Research Laboratory (PGRL) has helped researchers within and outside the department and has also served several industries in providing R&D support. The Unit Operations Lab (now known as Jeet Bindra Unit Operations and Innovation Lab) has also been completely upgraded and renovated with support in the form of generous donation by our alumnus, Shri Jagjeet Singh Bindra .

With several notable alumni spread across the globe, the Department’s remarkable history is alive and continue to make an impact in research labs, industry, and universities around the world. Hopefully this brief view conveys the essence of our history and current direction.

Academic Programmes

The department offers the PhD and MTech (2 year) programs at the PG level and the BTech (4-year) program at the UG level. The UGs also have the option of converting to the 5-year dual (BTech + MTech) program in the first three years of their program.

Engineering new biomaterials, developing catalysts and processes for sustainable energy, improving methods for drug delivery, creating safer, more environmentally friendly plastics-whatever passion a student might have, a diverse array of options are available to students pursuing UG & PG degrees in Chemical Engineering@IITK, including wide-ranging opportunities in the biotechnology, biochemical, environmental, chemicals and energy sectors. Students conduct research with renowned faculty to develop processes that use environmentally friendly materials and consume less energy, manufacture products to improve human health and solve the grand challenges facing the world.

1. Undergraduate Program

Bachelor of Technology (BTech) & BTech -MTech Dual Degree:

The undergraduate program in Chemical Engineering offers a sequence of courses beginning in the first year and extending through the senior years. The fundamental analytic tools of chemical engineering—chemical kinetics, chemical thermodynamics, and fluid mechanics—are developed in the second and third years. These tools are used to analyse the units of chemical processes: chemical reactors, bio-reactors, distillation columns, and heat exchangers. As per the latest curriculum, the students can opt for the MTech program in their third year and thereby earn a dual degree at the end of 5 years. Thus, the dual degree program can be completed within a single year after the bachelor's degree. The curriculum allows students to take a variety of elective courses that exposes them to the current trends of the profession. It is designed such that there is enough flexibility to either opt for advanced level courses or explore internship opportunities or even pursue entrepreneurial activities. BTech students are encouraged to involve themselves in short-term research projects, working alongside MS and PhD scholars in various groups, as well.

2. Postgraduate Program

The department offers a Master of Technology (MTech), MS (By Research) and a Doctorate (PhD) degree in Chemical Engineering. These programs are research centric and prepare the student for a productive research career. The rigorous course work and research provide a healthy balance of breadth in ChE fundamentals and depth in their chosen research field.

Master of Technology (MTech) & MS (By Research):

These 2 year programs enable new as well as practicing engineers to earn professional degrees while building expertise in related fields. The diverse personal and academic backgrounds of our faculty and students, and our vast facilities, make these exceptional programs. These professional degrees gives students the opportunity to:

- gain specialized focused knowledge in areas central to chemical engineering.
- deepen their knowledge of one topical area related to chemical engineering by specializing in an area of study, such as polymers, electronic materials, engineering management, food engineering, etc.
- broaden their skills (e.g., take courses in finance, marketing, language proficiency, entrepreneurship, etc.).
- undertake original research in one of the faculty research projects.

Doctor of Philosophy (Ph. D.)

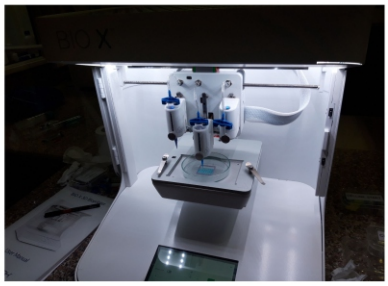
The PhD programme in chemical engineering will prepare the students for careers in academia and research. It is designed to prepare each student to participate in technology development, problem solving and innovation in chemical engineering, be it in industry, research institutions and universities. Students can enter the PhD programme either with a master's or a bachelor's degree in engineering. In the PhD programme, each student selects a research advisor and plans a programme of course work and thesis research. Independent research work is assessed by a comprehensive examination midway in the programmes and annual assessments thereafter culminating in a defense of the thesis at the end.


TECNAI

Areas of Research

The department is well known for its expertise in conventional areas of chemical engineering such as process engineering, process simulation, optimization and control, separation process, polymer engineering and transport phenomena. We have kept ourself abreast with technological developments and needs by taking up challenges in new areas of chemical engineering such as nanotechnology, carbon capture, utilization & sequestration, machine learning, etc. Our research may be categorised into six basic themes as below, which are briefly overviewed.

- Materials and Nanotechnology
- Complex fluids and Soft Matter
- Catalysis and Reaction Engineering
- Energy and Sustainability
- Theory, Computation and Machine Learning
- Biotechnology and Bio-systems



Materials and Nanotechnology

Nanoscience and technology today is an emerging research area that aims at developing new generation of materials and devices engineered at the nanoscale for ground breaking properties and functionalities for diverse applications such as drug delivery, diagnostics, electronics, cosmetics and catalysis. Control of matter at the nanoscale is crucial for imparting properties, shapes and chemical compositions that are very different from their bulk counterparts. Fundamental properties - such as quantum properties, solubility and surface chemistry can thus be engineered to make the materials suitable for specific applications. Ours is one of the leading departments in nanoscience and technology research endowed with state-of the- art research facilities. The mission is to develop highly innovative materials and products for society via innovation. Currently, six faculty members are involved in nanoscience and nanotechnology research projects with multidisciplinary research efforts. Several projects have been funded by government agencies (e.g. DST, DBT, DRDO, BRNS, etc.) as well as industries (e.g. Chevron, HLL, etc.).

Our current research encompasses nanolithography, nanosensors, nano-drug delivery, sustainable energy materials and systems, nanoadhesives, functional polymers, self assembly, nanowires, nanocarbon materials, nanocomposites, carbon MEMS, nanocatalysts, nanosoftmaterials, nanotribology, lab on chips, nanophosphors, nanomechanics, etc.

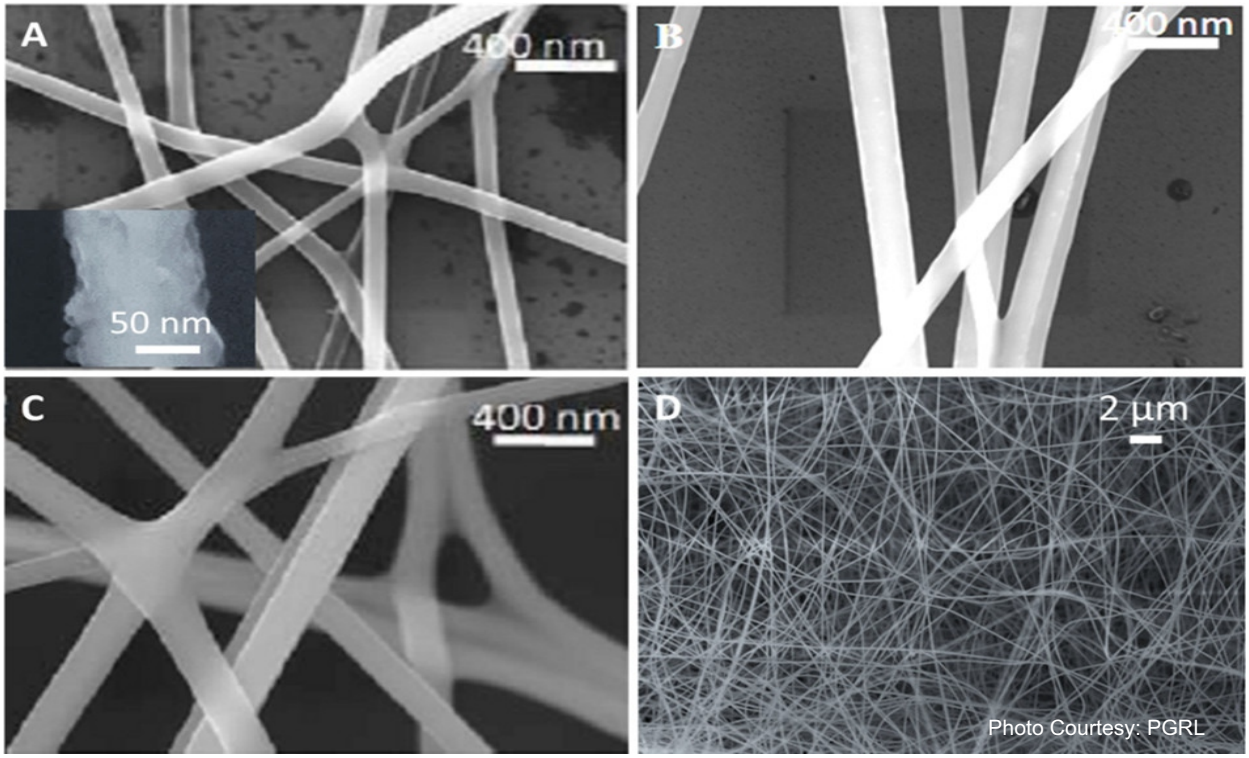


Photo Courtesy: PGRL

Complex fluids and Soft Matter

Complex fluids are multiphase systems comprising of a continuous phase and a dispersed phase. Typical examples include polymer solutions and melts, colloidal suspensions, emulsions, foam, etc. Many food items, pharmaceuticals, cosmetics involve complex fluids during their processing or in their end product. Due to the presence of a dispersed phase, whose length scale is large compared to molecular scales, the structure and flow behaviour of complex fluids are dramatically different from simple (Newtonian) fluids, such as water and air.

At IIT Kanpur, the Department of Chemical Engineering focuses on a diverse class of problems spanning both fundamental and application aspects of complex fluid behaviour. An ongoing work in this area is on thixotropic and soft-glassy rheology with applications aimed at processing of pasty materials in fertilizer, food, and consumer goods industries. Another emphasis has been to elucidate the role of non-Newtonian rheology on the transition from laminar to turbulent flow states in the flow of polymer solutions. Similarly, an ongoing work aims to understand the transport of complex fluids in porous media for energy and environment applications. Department is also venturing in exploring soft materials based on polymeric elastomers tailored with microstructures to form novel adhesives with potential application in healthcare. A recent interest is in Active colloids/emulsions, wherein, the dispersed phase colloids/droplets undergo spontaneous, yet directed motion via self-propulsion. These systems serve as model systems to understand the dynamics of several biological processes and carry futuristic application in biomedicine and environmental remediation. Our department utilizes state-of-the-art experimental techniques and analytical techniques (theory and simulations) to venture into these diverse problems related to polymers and complex fluids.

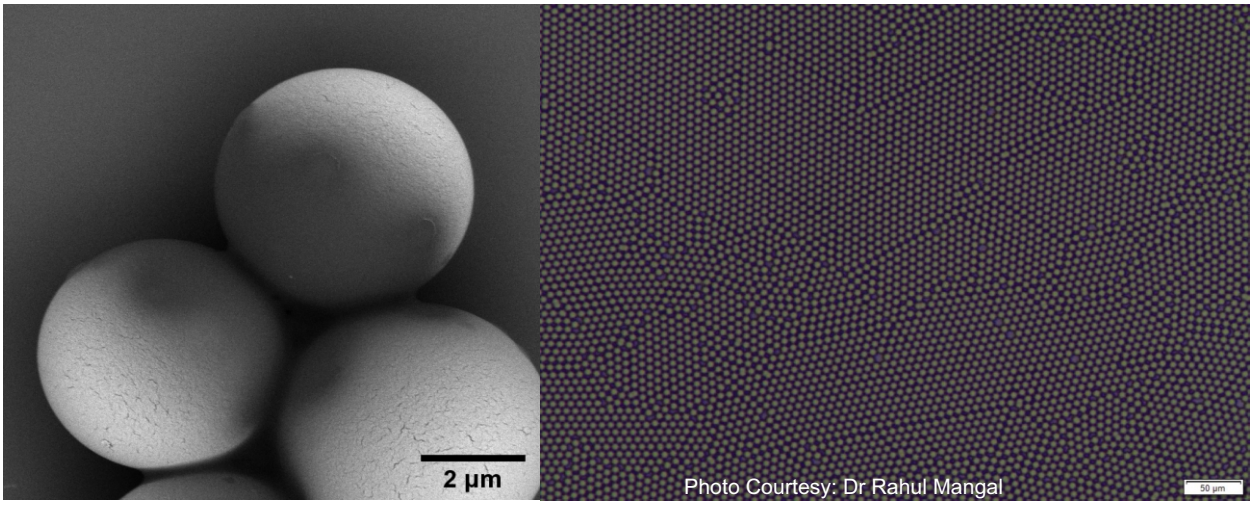


Photo Courtesy: Dr Rahul Mangal

Catalysis and Reaction Engineering

The Catalysis and Reaction Engineering group at the Chemical Engineering Department, IIT Kanpur is actively involved in understanding the science and engineering across different length and time scales for various environmentally friendly catalytic processes. Applications range from thermo-catalytic to electro-catalytic and solar-catalytic processes. These reactions include those of recent interest, such as bio-mass conversion, carbon dioxide conversion, and oxygen-, chlorine- and hydrogen- evolution reactions, and those that are traditionally applied in the chemical process industry, such as hydrodesulfurization and various methane reforming reactions. Catalytic reactions for sustainable energy production are also in the forefront. Molecular level understanding of catalytic reactions is achieved through atomistic simulations, such as density functional theory (DFT), and mechanistic insights are developed through a combination of multi-scale computational and experimental techniques. Novel catalyst formulations, mechanistic interrogations, and reactor development are pursued by different groups to address societal needs.

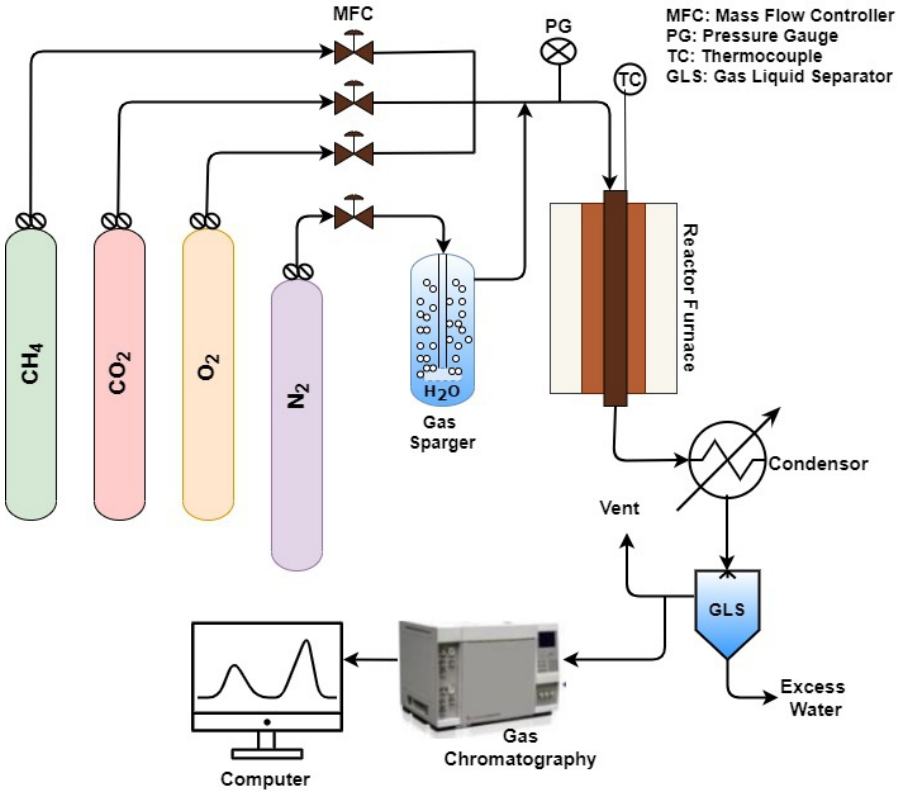


Photo Courtesy: Dr Goutam Deo

Energy and Sustainability

Today energy and environment are arguably the two principal challenges facing mankind in its quest for sustainable development. Obtaining energy in an environmentally sustainable manner provides a unique challenge and opportunity for chemical engineers. Our focus is on chemical, electrochemical and photoelectrochemical methods of energy capture, storage and conversion utilizing the synergy between phenomenological modelling and systematic experimentation. The energy research portfolio encompasses experimental work on development and characterization of solid oxide and charged ultrafiltration membrane fuel cells, in-situ H_2 generation and storage, electrochemical batteries, photovoltaic and tailored nano/microcatalysts for specific process applications. In addition, quantum chemical density functional theory, molecular dynamics, Monte Carlo methods and continuum transport modelling approaches are applied for developing a fundamental understanding of relevant phenomena at different scales and applying these tools for synthesizing functionally superior materials for energy capture, storage and conversion. The department is actively engaged in carrying out fundamental as well as applied research towards developing green technologies. These range from the synthesis of carbon nanofibers and carbon nanoparticles based adsorbents and catalysts for air and water remediation, to the design and development of novel membrane separation techniques for the treatment of industrial effluents and the development of silicon and conducting polymer based chemical sensors for environmental pollution monitoring. Several industrial and government sponsored projects support the various research activities related to the technology development in air and water pollution monitoring and abatement. Areas of major research focus are Renewable, low-carbon heating, cooling and power technologies, Integrated energy systems, Carbon capture, utilisation and storage, Waste management, Life-cycle assessment, Sustainable manufacturing and multi-objective optimisation.

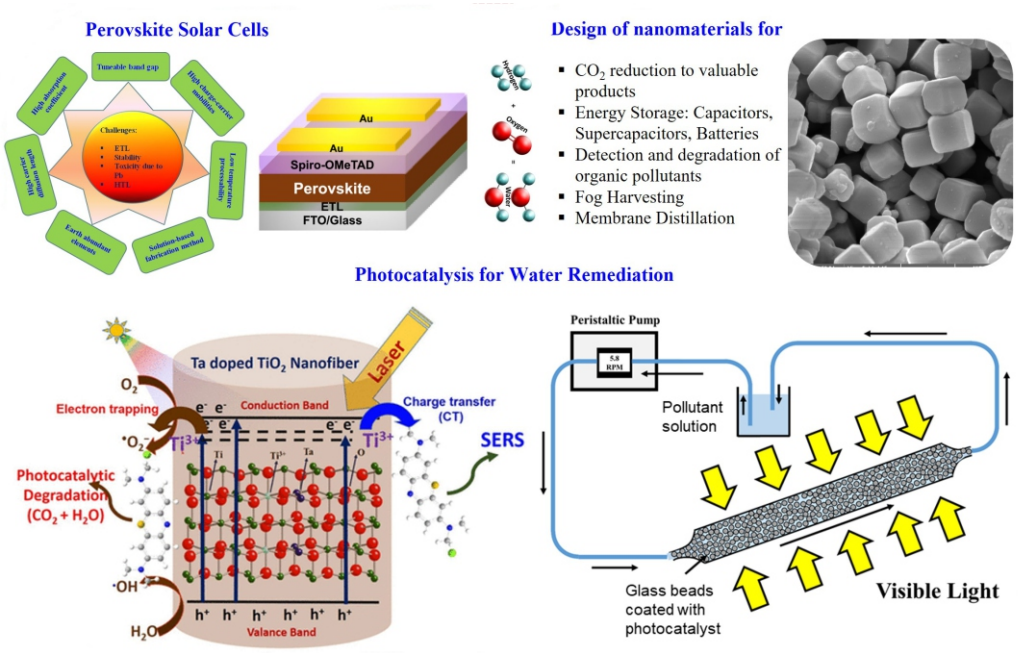


Photo Courtesy: Dr Raju K. Gupta

Theory, Computation and Machine Learning

Several of our faculty members are involved in doing fundamental research using theoretical and numerical tools. Some of the examples involve predicting laminar to turbulent transition in pipe flows for complex fluids, pattern formation in thin film flows due to instability, models to understand cell biology, etc. The computational techniques and methods employed and/or developed vary from electronic to continuum levels.

Molecular simulations have become a powerful tool to understand and predict the structural, thermodynamical, and dynamical properties of materials. Our department has exceptional depth and breadth in the area of statistical mechanics methods and molecular simulation techniques ranging from quantum chemistry to molecular dynamics, Monte Carlo, and coarse-grained methods. Several of our faculty also work in the area of multiscale simulations. The materials being investigated include soft materials, such as polymers and colloids, ionic materials, composite materials, semiconductors, metals, and liquid systems. The emphasis on developing a fundamental understanding of a range of problems, such as understanding the thermodynamic aspects of phase transitions in the condensed phases; the effect of polar, hydrogen bond, and hydrophobic interactions on the structural and dynamical phenomena at the nanoscale; self-assembly in soft condensed, and design of new catalysts.

Few of us are utilizing machine learning/AI methods to accelerate the learning and discovery of materials such as suitable MOF for carbon capture or catalyst for CO_2 conversion. The goal is to develop tools that integrate different AI/ML with molecular simulation methods, to accelerate learning, rationale design of materials, and create a pipeline for high-throughput screening of materials/molecules.


Photo Courtesy: Computer Centre

Biotechnology and Bio-systems

Research in Biosystems Engineering is primarily focused on the following themes namely, (i) Biomimetic Engineering (ii) Engineered Nanoparticles for biological applications (iii) Computer Aided Product and Process Design (iv) Systems Biology.

In the area of Biomimetic engineering, inspired by the unique physical characteristics and exceptional functional abilities of naturally adhesive surfaces, research groups in the department have explored the effect of geometry of surface patterns, softness of materials and resultant deformation in them by variety of forces including those induced by solid-liquid interfacial interactions. Researchers here have designed hierarchically structured adhesives, ones having viscoelastic inclusions, adhesive layers embedded with liquid filled channels thereby mimicking adhesive pads of organisms containing fluidic vessels and air pockets. In the area of engineered nanoparticles for biological applications, the group has been focusing on designing of a novel class of multifunctional nanoparticles (e.g. polymer nanoparticles/capsules, metal, magnetic, semiconductor, and lanthanide-doped nanoparticles) for variety of bioapplications such as magnetic resonance imaging (MRI) contrast agents, drug delivery vehicles, biolabels, and biosensors. Work in the area of Computer aided product and process design focuses on health and environmental applications using molecular biology and mathematical programming e.g. the aim of one of the projects in this theme is to evaluate small interfering RNAs (siRNA) as a therapeutic for the Alzheimer's disease (AD) using in silico and in vitro frameworks. The major aim of another project is to develop a novel wastewater treatment technology using recombinant bacteria for source point application. In the area of Systems Biology, the group is working towards understanding the complex interactions between the transcription network and signaling network. In biosystems, researchers here are interested in the underlying mechanism of many such phenomena. For example, especially in cancer, homeostasis of the tissue is important and can be perturbed by changes that occurs in signaling and transcription network.

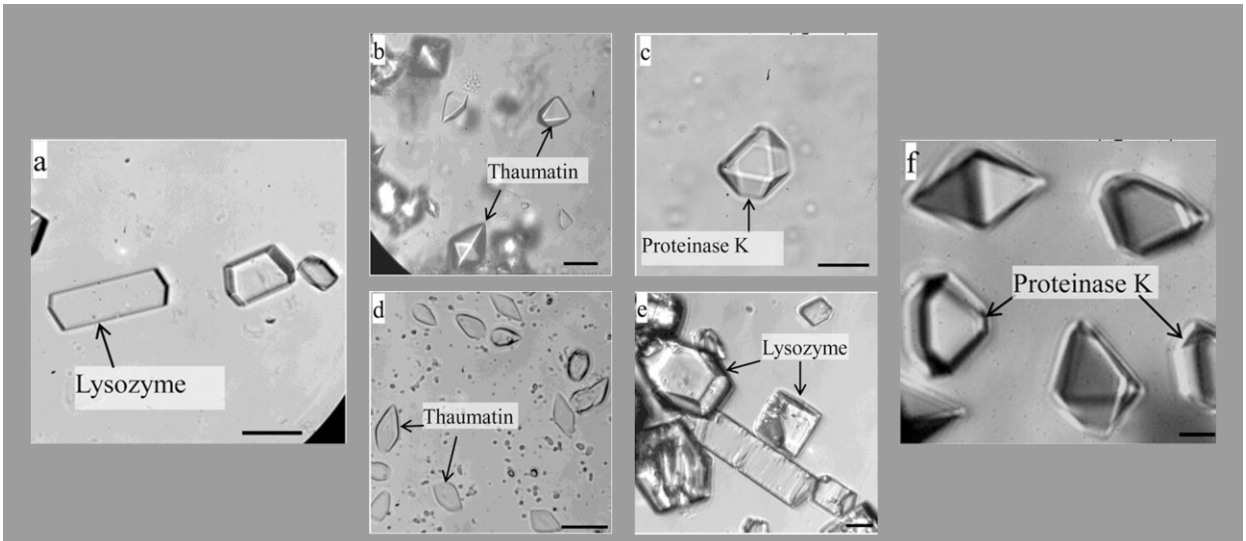


Photo Courtesy: Dr Animangsu Ghatak

2022 Graduating Batch of Chemical Engineering @ IIT Kanpur with faculty members and institute's special convocation day guest Ms.Vartika Shukla, ChE Alumni & Current Chairman & Managing Director of Engineers India Limited (EIL)

Research Themes of Faculty

Faculty	Materials And Nanotechnology	Biotechnology and Bio-systems	Catalysis and Reaction Engineering	Complex Fluids and Soft Matter	Energy and Sustainability	Theory, computation and Machine learning
Dr. Akash Choudhary				★		★
Dr. Animangsu Ghatak	★	★		★		
Dr. Anurag Tripathi				★		★
Dr. Ashutosh Sharma	★			★		★
Dr. Dipin Sasidharan Pillai				★		★
Dr. Goutam Deo			★			
Dr. Harshwardhan Hemant Katkar				★		★
Dr. Himanshu Sharma				★	★	
Dr. Indranil Saha Dalal				★		★
Dr. Ishan Bajaj					★	★
Dr. Jayant Kumar Singh	★			★	★	★
Dr. K. P. Krishnaraj				★		
Dr. Naveen Tiwari				★		★
Dr. Nishith Kumar Verma	★			★	★	
Dr. Nitin Kaistha				★	★	★
Dr. Pankaj Arvind Apte			★			★
Dr. Raghavendra Ragipani					★	
Dr. Raghvendra Singh		★				
Dr. Rahul Mangal				★		★
Dr. Raj Ganesh Santharam Pala			★		★	★
Dr. Raju Kumar Gupta	★				★	
Dr. Sanjeev Garg		★				
Dr. Siddhartha Panda	★				★	
Dr. Soumik Das	★			★		
Dr. Sri Sivakumar	★	★				
Dr. Vishal Agarwal			★		★	★
Dr. Viswanathan Shankar				★		★
Dr. Yogesh Moreshwar Joshi	★			★		★

Mr. Rahul Gautam, CMD, Sheela Foam Ltd delivered PetroTel Distinguished Lecture 2022
Talk Title : Helping India Sleepwell – Life Story of an IIT Kanpur Chemical Engineer

Faculty Profiles

Akash Choudhary

Assistant Professor

PhD, IIT Madras
Contact: Ph No: +91-512-679-2386
Email: achoudhary@iitk.ac.in
Web: https://www.iitk.ac.in/che/achoudhary.html

Awards and Honours:

- Alexander von Humboldt fellowship for postdoctoral research (2020)
- Scholarship for Côte d'Azur University Fall program on Complex Systems (2021)

Research:

Numerous natural and industrial processes involve systems of particles suspended in fluids. Active suspensions, however, are distinguished from these systems as they are driven out of equilibrium through either external forces or self-propulsion, resulting in a deliberate and organized movement. Such systems are represented by motile microorganisms and motor-protein in the cytoskeleton, which are pervasive in living beings and natural habitats. Their artificial counterparts, active colloids, translate in potential or chemical gradients, generated either externally or internally via asymmetry in surface properties. Due to this localized energy-work conversion, these systems exhibit unusual macroscale properties that are in stark contrast to passive suspensions; for instance, enhanced diffusion, reduction of effective viscosity, and generation of normal stresses. Fluids and particles can also be driven via externally applied potential or chemical gradients that have applications at the micro and nanoscale. The suspended matter is thus subjected to evolve over a certain time scale enforced by the gradients in flow or chemical potential, relevant to the application. Competition with the inherent time scales of the activity of suspended matter can yield emergent properties. Our research group aims to model and predict the behaviour of such systems at two length scales:

(i) Microscopic view: How do these additional time scales alter the hydromechanics and navigation strategies of motile pathogens and artificially active colloids? What dominant mechanisms govern the orientational dynamics in sheared flows and how they interact with other swimmers and boundaries? And how does all this alters in biologically relevant non-Newtonian media?

(ii) Macroscopic view: What is the impact of these competing time scales on the rheological response, suspension stability, and spatiotemporal patterns?

Our group utilizes both analytical and computational techniques to gain fundamental insights. The former tools exploit the separation of time/velocity scales in the system and consist of asymptotics & perturbation techniques, and integral representation of experimentally measurable quantities. These provide handy expressions that can be readily used by experimentalists. However, these are mostly valid under limiting conditions. Thus, computational techniques based on finite difference or harmonic expansion of unabridged transport equations and mean-field kinetic models offer a more comprehensive understanding. Furthermore, motivated by the ubiquity of collective motion and the spreading of microbial systems, our group is also developing particle-based simulations governed by overdamped Langevin dynamics.

Selected Publications:

1. A. Choudhary, S. Paul, F. Ruhle, H. Stark, How inertial lift affects the dynamics of a microswimmer in Poiseuille flow, Communications Physics, 5, 14 (2022).

2. A. Choudhary, H. Stark, On the cross-streamline lift of microswimmers in viscoelastic flows, Soft Matter, 18 (2022).

Animangsu Ghatak

Professor

C. V. Seshadri Chair Professor
PhD, Lehigh University
Contact: Ph No: +91-512-259-6045
Email: aghatak@iitk.ac.in
Web: https://home.iitk.ac.in/~aghatak

Awards and Honours:

- SERB - Science and Technology Award for Research (SERB-STAR) (2020)
- Fellow of Indian National Academy of Engineering (2018)
- C. N. R. Rao Faculty Award, IIT Kanpur (2016)
- DOST Professor S. K. Sharma Medal and Chemcon Distinguished Speaker Award (2015)
- Gireesh Jankinath Chair, IIT Kanpur (2014-2017)

Research:

Highly deformable, soft elastic, viscoelastic and poroelastic materials occur in many different fields of research, e.g. adhesives, therapeutic patches, shock absorbers, dampeners, platforms for micro-fluidic devices, biomaterials, prosthetic devices, in biology as soft tissues, stems, roots and leaves, sponges, cartilage layers and in cutting-edge research fields like soft robotics, wearable electronics, conforming interfaces for biological surfaces and so on. In these variety of applications these materials are subjected to many different forms of mechanical loads, e.g. tension, compression, torsion, bending; apart from surface traction, these materials are subjected to also different body forces, e.g. electric and magnetic field. Due to the large deformability, their specific geometrical features and complex rheological character, these materials respond differently from that commonly observed with linear elastic materials. In our laboratory, we study gels, elastomers, composites of solid-liquid and solid-solid two phase materials in the context of wetting, adhesion, friction, fracture and failure. We have particularly examined the effect of surface energy and surface tension on above problems, variety of solid-solid and solid-liquid interfacial effects, deformation induced by surface tension of solid and liquid, combined effect of geometry and surface energy such deformation, instability in solid induced by confinement, confinement induced morphological phase transitions in complex emulsions, mixing at low Reynolds at the confined geometry of microfluidic channels, effect of geometry on fracture toughness of a soft material and so on.

Selected Publications:

1. A. Ghatak, How does a lizard shed its tail?, Perspective article in Science, 375, 721 (2022).
2. N. Singh, A. Ghatak, Hierarchically Rough Surface used as Rewritable and Reprintable paper, arXiv preprint arXiv:2111.12430 (2021).
3. K. K. Kuhar, M. Jesbeer, A. Ghatak, Soft gel-filled composite adhesive for dry and wet adhesion, ACS Applied Polymer Materials, 3, 3755 (2021).
4. N. Singh, Y. Jain, K. Kishore, A. Ghatak, Liquid spreading induced by in-situ generation of metallic nano-particles, Langmuir, 36, 12237 (2020).
5. K. K. Kundan, A. Ghatak, Fingering instability during fracture of a gel block subjected to shear loading, Physical Review E, 102, 013002 (2020).
6. P. Rajbanshi, A. Ghatak, Analysis of mixing in helical micro-channel, Physical Review Fluids, 5, 064502 (2020).

Anurag Tripathi

Associate Professor

PhD, IIT Bombay

Contact: Ph No: +91-512-259-6591
Email: anuragt@iitk.ac.in

Web: https://sites.google.com/view/anuragtripathi/home

Awards and Honours:

- Award of Excellence in Ph.D. Thesis in the Department of Chemical Engineering, IIT Bombay (2009-2011)
- Travel grant award from American Physical Society-Division of Fluid Dynamics (APS-DFD) for attending 63rd Annual Meeting of APS-DFD 2010 at Longbeach, CA (2010)

Research:

Our research group focuses on understanding the behaviour of bulk solids with a special focus on granular materials. This category of substances consists of numerous distinct solid particles. Examples include grains, cereals, pulses, sand, coal, etc. Though encountered commonly in a variety of natural and industrial settings, understanding and predicting their flow and mixing behaviour is a challenge. The varied flow behaviour that these substances can display contributes to the difficulty of predicting their behaviour. Investigating the rheology of granular materials in these different flow regimes is an active area of research in our group. Using discrete element method simulations, we obtain the constitutive equations that can accurately describe the flow of granular materials in different regimes. The flow behaviour and rheology of cohesive and wet granular materials is also being investigated.

Another aspect of our research is aimed at understanding and predicting the mixing and segregation phenomena in granular mixtures. The fundamental understanding of segregation of binary mixtures due to difference either in density or in size based on computation of particle level forces by our group enables accurate predictions of various flow properties of interest in simple shear flows. Combined effect of size and density difference on segregation of mixtures are currently being investigated. In addition, efforts to extend the theory for predicting flow and segregation of multi-component mixtures are being pursued.

Quantitative simulations of powders and other bulk solids for existing industrial operations/equipment is another focus area of our research. A systematic approach, utilising direct experimental measurements of particle level properties using table top experiments, image processing as well as those at the level of the bulk material enable determination of various DEM parameters for quantitative simulations and significantly reduce the number of iterations required using the popular trial-and-error method of bulk calibration.

Selected Publications:

1. S. Patro, M. Prasad, A. Tripathi, P. Kumar, A. Tripathi, Rheology of two-dimensional granular chute flows at high inertial numbers, Physics of Fluids, 33, 113321 (2021).

2. A. Tripathi, A. Kumar, M. Nema, D. V. Khakhar, A theory for size segregation in flowing granular mixtures based on computation of forces on a single large particle, Physical Review E, 103, L031301 (2021).

3. K. A. Kumar, D.V. Khakhar, A. Tripathi, Soft Theoretical calculation of the buoyancy force on a particle in flowing granular mixtures, Physical Review E, 100, 042909 (2019).

Ashutosh Sharma

Professor

Institute Chair Professor
PhD, State University of New York at Buffalo
Contact | Ph No: +91-512-259-7026
Email: ashutos@iitk.ac.in
Web: https://home.iitk.ac.in/~ashutos/

Awards and Honours:

- Dr. B P Godrej Life Time Achievement Award (2022)
- President, Indian National Science Academy (2022)
- Institute Fellow (2020)
- UNESCO Medal for outstanding scientific contributions to the development of nanoscience and nanotechnologies (2017)
- Distinguished Alumni Award, State University of New York, SUNY Buffalo (2016)
- MRSI Distinguished Lectureship Award, Materials Research Society of India, (2011-12)
- Syed Husain Zaheer Medal, INSA (2011)
- Infosys Prize in Engineering and Computer Science (2010)
- Fellow, Indian National Academy of Engineering (2009)
- The TWAS Prize in Engineering Sciences, Italy (2008)
- Friedrich Wilhelm Bessel Research Award, Alexander von Humboldt Foundation (2006)
- J. C. Bose National Fellowship, Department of Science & Technology (2006)
- Fellow, Indian National Science Academy (2004)
- Herdillia Award of the Indian Institute of Chemical Engineers for excellence in basic research (2003)
- Shanti Swarup Bhatnagar Prize in Engineering Sciences (2002)
- Fellow, Indian Academy of Sciences (1999)
- Fellow, National Academy of Sciences, India.

Research:

Research in Prof. Ashutosh Sharma's group mainly focusses on: understanding and control of interfacial instabilities in soft, highly confined visco-elastic materials with applications in the meso-scale patterning and micro-nano fabrication by self-organization. Some recent examples of self-organized patterning of thin films are by dewetting, adhesion, external fields and laser diffraction. Other related themes include multiscale functional interfaces and nanomaterials in applications ranging from structured adhesion and wetting to multiscale polymeric and carbon based structures used in microfluidic, MEMS, Sensors, energy, environment and health.

Selected Publications:

1. N. Bhandaru, N. Agrawal, M. Banik, R. Mukherjee, A. Sharma, Hydrophobic recovery of cross-linked polydimethylsiloxane films and its consequence in soft nano patterning, Bulletin of Materials Science, 43, 186 (2020).

2. V. Mohania, T. D. Deshpande, Y. R. G. Singh, S. Patil, R. Mangal, A. Sharma, Fabrication and characterization of porous poly(dimethylsiloxane)(PDMS) adhesives, ACS Applied Polymer Materials, 3, 130 (2020).

3. B. Mordina, R. Kumar, N. S. Neeraj, A.K. Srivastava, D. K. Setua, A. Sharma, Binder free high performance hybrid supercapacitor device based on nickel ferrite nanoparticles, Journal of Energy Storage, 31, 101677 (2020).

4. T. D. Deshpande, Y. R. G. Singh, S. Patil, Y. M. Joshi, A. Sharma, Adhesion strength and viscoelastic properties of polydimethylsiloxane (PDMS) based elastomeric nanocomposites with embedded electrospun nanofibers, Soft Matter, 15, 5739 (2019).

Dipin S. Pillai

Assistant Professor

PhD, IIT Madras
Contact: | Ph No: +91-512-259-2108
Email: dipinsp@iitk.ac.in
Web:https://home.iitk.ac.in/~dipinsp

Awards and Honours:

- Institute Research Award for excellence in research during Ph.D., IIT Madras (2015)

Research: Our group works on leveraging interfacial science and instabilities to enhance transport in diverse technologically relevant areas. A prominent aspect of our research involves developing reduced-order models for physico-chemical transport processes to gain analytical or semi-analytical insights. Some of our recent efforts have been aimed at developing fundamental understanding of wetting alteration using electric fields, investigating the origin of self-assembled pattern formation in porous anodic oxides, non-linear dynamics of liquid jet breakup, as well as development of theoretical models for active swimming droplets.

Wetting alteration by electric field, known as electrowetting, is a complex interfacial phenomenon associated governed by the statics and dynamics of the triple phase contact line. A comprehensive understanding of this phenomenon has implications in liquid displays, electrospraying, as well as droplet microfluidics. In droplet-based microfluidics, incorporation of external electric field provides control over mixing, transport and manipulation of droplets. Our group has recently developed reduced-order models for electrified sessile droplets of varying physical and electric properties under steady and periodic fields. The behaviour of surfactant-infused droplets is also of interest as most biological assays involve surface active agents such as macromolecular proteins. We also employ the tools of calculus of variation (CV), and molecular dynamics simulations to arrive at deeper understanding of the phenomenon of electrowetting.Surface oxide films are formed on metals such as aluminum, titanium, and tantalum, during oxidation in electrochemical cells, a process known as anodization. Under the right conditions, films can be obtained with highly regular arrangements of pores with submicron diameters. Numerous devices for energy, optical, catalytic, and biological applications make use of porous anodic oxide (PAO) films, taking advantage of their high specific surface area. Our group focuses on revealing the fundamental interfacial reactions and ion migration processes associated with anodization, and the electrochemical factors defining the geometric and chemical structures of PAOs. Liquid jets are encountered in several applications such as inkjet printing, fuel injectors, spray painting, oil transportation, and microfluidics. A liquid jet breaks up into drops as the system evolves minimizing the free energy- an example of interfacial instability known as the Rayleigh-Plateau instability. Often the break-up of jets results in the formation of primary and satellite droplets, leading to intriguing non-linear dynamics. The single-period breakup of a jet into primary droplets as well as its period-doubling leading to the formation of satellite droplets are influenced by the thermophysical properties of the liquid jet as well as the presence of any impurities such as surfactants. A reduced-order model to lay bare the complex non-linear dynamics of surfactant-laden liquid jet breakup is currently being developed.

Selected Publications:

1. M. A. Kainikkara, D. S. Pillai, K. C. Sahu, Equivalence of sessile droplet dynamics under periodic and steady electric fields, npj Microgravity, 7, 1 (2021).

2. D. S. Pillai, K. C. Sahu, R. Narayanan, Electrowetting of a leaky dielectric droplet under a time-periodic electric field, Physical Review Fluids, 6, 073701 (2021).

Goutam Deo

Professor

PhD, Lehigh University
Contact: | Ph No: +91-512-259-7881
Email: goutam@iitk.ac.in
Web:https://home.iitk.ac.in/~goutam

Research: The research in our group is aimed on understanding the activity and selectivity relationships for supported metals and metal oxides catalyst for a variety of reactions. The reactions that are currently being targeted are the CO_2 utilization reactions, which include the CO_2 assisted methane reforming and associated reforming reactions for syngas production. The CO_2 reforming of methane, where the reforming of methane takes place in the presence of CO_2 instead of the commonly used steam (H_2O), is commonly referred to as the dry reforming of methane (DRM). The disadvantages associated with the DRM reaction are addressed by developing more active and stable catalysts, e.g., by using promoted catalysts; and by modifying the operating conditions of the process, e.g., by using high temperatures and/or limited amounts of oxygen as in the oxidative dry reforming of methane (ODRM). We are exploring the possibility of using this knowledge for the reforming of methane using flue gas, which is also a source of CO_2 along with N_2, H_2O, O_2 and other minor components. Without separating CO_2, we have shown that syngas can be produced. Consequently, harmful flue gas emissions can be used to produce value-added products by using the flue gas reforming of methane (FGRM) process. Since these reforming reactions are highly exothermic, the advantage of depositing these catalysts on structured reactors are also being explored. Previously, we successfully tested structured reactors for the steam reforming of methane using an active nickel-based catalyst and believe that we can apply the same to the currently studied reforming reactions. Simultaneously, the experimental values of the reactivity of the catalysts for the different type of methane reforming reactions are simulated by microkinetic modelling and rate expression are being developed. Conditions for achieving optimum methane conversion and hydrogen production rates have been proposed. Development of microkinetic models for promoted nickel catalysts are being attempted. The other CO_2 utilization reaction is the traditional Sabatier reaction, where CO_2 and CO are hydrogenated to methane. This reaction has several applications, which include those in the traditional chemical industry as well as for space. We are currently trying to synthesize an active catalyst that will be useful for carrying out the hydrogenation of CO_2 to methane. Concurrently, we are developing rate expressions from the experimental data of various catalysts, which will assist us in designing and analysing a suitable micro-reactor. As in the methane reforming reactions, the optimized catalyst will be deposited on structured reactors to enable efficient heat and mass transfer and improved selectivity of methane. Catalyst development for the CO_2 assisted propane to propene conversion is another CO_2 utilization reaction that is being investigated. Development of an active catalyst will assist in the simultaneous production of propene and utilization of CO_2. To achieve all the above goals we synthesize, characterize and test the catalysts for the above reactions. A judicious choice of synthesis and characterization techniques complimented with reactivity data assists in improving our understanding of several of these systems, which is essential for the development of efficient catalysts for the targeted reaction.

Selected Publications:

1. P. Chaudhary, G. Deo, Role of metal-support interaction on the catalytic performance of Ni-Al_2O_3 catalysts for the dry and oxidative-dry reforming of methane, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 646, 128973 (2022).

2. A. S. Russel, P. Chaudhary, P. Jain, G. Deo, Microkinetic and sensitivity analysis of oxidative dry reforming of methane on Ni-Co catalyst using a reaction mechanism based on Ni, Reaction Chemistry & Engineering, 6, 2104 (2021).

Harshwardhan H. Katkar

Assistant Professor

PhD, University of Massachusetts Amherst

Contact: | Ph No: +91-512-259-2095
Email: hkatkar@iitk.ac.in

Web:https://home.iitk.ac.in/~hkatkar

Research:

The overarching theme of reasearch activities in the group is to develop a fundamental understanding of important biological polymers and assemblies, and to develop engineering solutions for an improved healthcare. We are interested in employing multiscale modeling and simulation tools, systematic coarse-graining strategies and enhanced sampling techniques to enable designing of nanopores for accurate diagnosis of diseases, identifying of novel drug targets and improving drugs and drug-carriers for treating diseases. We often use computational tools such as homology modeling, elastic network modeling and metadynamics to study the structure, interactions and dynamics of macromolecules, including biopolymers such as proteins and DNA. A major fraction of the burden on healthcare, worldwide and in India, is due to Tuberculosis (TB). There is a dire need to expand the limited set of TB drugs. Inspired from a recent experimental discovery, we are using computational tools to augment our understanding of the structure and dynamics of a large protein complex that is essential for the survival of the TB-causing bacterium. Our long term goal is to use this understanding to provide principles for rational design of drugs for TB and other infectious diseases. Changes in the structure of proteins and their aggregation are markers of several health disorders. Cost-effective and accurate detection of such diseases is important for personalized and timely medical intervention. Recent experiments have demonstrated the potential use of nanopores for this purpose. We are using theory and computational tools to discover principles that will guide the design of nanopores with essential surface modifications to detect structural changes in proteins. Further, identifying key interactions that drive aggregation or assembly of proteins and other macromolecules is relevant in rational design of drugs and in drug targeting. We are studying emerging collective behavior of macromolecular assemblies and their tunability through inter-molecular interactions using molecular dynamics and coarse-grained simulation. We are also interested in understanding the single-molecule-level effects of external flow and electric fields in these systems.

Selected Publications:

1. S. Mani, H. H. Katkar, G. A. Voth, Compressive and tensile deformations alter ATP hydrolysis and phosphate release rates in actin filaments, Journal of Chemical Theory and Computation, 17,1900 (2021).

2. V. Zsolnay, H. H. Katkar, S. Z. Chou, T. D. Pollard, G. A. Voth, Structural basis for polarized elongation of actin filaments, Proceedings of the National Academy of Sciences, 117, 30458 (2020).

3. F. Aydin, H. H. Katkar, G. A. Voth, Multiscale simulation of actin filaments and actin-associated proteins, Biophysical Reviews, 10,1521(2018).

4. H. H. Katkar, A. Davtyan, A. E. P. Durumeric, G. M. Hocky, A. C. Schramm, E. M. De La Cruz & G. A Voth, Insights into the cooperative nature of ATP hydrolysis in actin filaments, Biophysical Journal, 115, 1589 (2018).

5. H. H. Katkar, M. Muthukumar, Role of non-equilibrium conformations on driven polymer translocation, The Journal of Chemical Physics, 148, 024903 (2018).

Himanshu Sharma

Assistant Professor

PhD, University of Texas at Austin

Contact: | Ph No: +91-512-259-2073
Email: sharmah@iitk.ac.in

Web:https://home.iitk.ac.in/~sharmah

Research:

Our research group primarily works on flow of complex fluids through porous media and low-cost adsorbents for energy and environment applications. Fluid flow in porous media is relevant in various practical applications including enhanced oil recovery, ground water flow, geological Co_2 sequestration, etc.

The problems are interdisciplinary in nature and hold complexity at various scales. At the molecular scale, we are trying to understand the oil-brine-rock interactions leading to wettability alteration. Another problem of interest is to understand factors affecting the adsorption of surfactants during alkali-surfactant-polymer flooding. We complement these studies with flow studies at the lab scale to understand the effect of these molecular scale phenomena on multiphase flow. Consequently, we use a numerical simulator to upscale these (lab-scale) results to the field scale. We have recently developed an experimental facility for carrying out studies using realistic porous media at desired temperature and pressure conditions. Similarly, we have developed an in-house reservoir simulator for modeling two-phase flow with reactions. An ongoing study aims to understand factors affecting the wettability of natural porous media and its implications on multiphase flow. In our recent work, we investigated the role of organic acids, present in crude oil, and formation brine composition on the wettability of a carbonate surface. The study showed that divalent ions have a significant impact on rock wettability. Further studies are ongoing to understand the impact of rock wettability on multiphase flow. Along with experimental studies, we are also developing a multiscale reservoir simulator for modeling multiphase flow through porous media. Our in-house simulator is currently able to model two-phase flow with reactions, assuming local equilibrium, in one-dimension. The simulator is currently being extended to three-dimensions and more functionalities are being added. In another ongoing study, we are investigating the transport of polymers and nanoparticles in porous media; particularly, their transport in low permeability rocks.

Another key focus of our research group is on low-cost adsorbents for environmental applications; particularly carbon capture. Our preliminary work has resulted in the development of adsorbents for treating pharmaceutical waste. These adsorbents are being suitably modified for enhancing their capability for carbon capture.

Selected Publications:

1. S. Bind, H. Sharma, Effect of brine and organic acids on the initial wettability of carbonate rocks, Energy & Fuels, 36, 10123 (2022).
2. H. Sharma, K. K. Mohanty, Modeling of low salinity waterflooding in carbonates: Effect of rock wettability and organic acid distribution, Journal of Petroleum Science & Engineering, 208, 109624 (2022).
3. K. Panthi, H. Sharma, K. K. Mohanty, Oil-tolerant non-ionic worm like micellar solution, ACS Omega, 5, 30817 (2020).
4. K. H. Baek, R. Okuno, H. Sharma, U. Weerasooriya, Oil-in-water emulsification of Athabasca bitumen with pyrrolidine solution, Fuel, 246, 425 (2019).

Indranil Saha Dalal

Assistant Professor

PhD, University of Michigan
Contact: | Ph No: +91-512-259-6702
Email: indrasd@iitk.ac.in
Web:https://home.iitk.ac.in/~indrasd

Awards and Honours:

- Teaching Excellence award, IIT Kanpur (2022)
- DST Early Career Research Award (2017)
- Ivor K. McIvor Award, University of Michigan (2012)

Research:

The research in our group spans various areas of theory and simulations of complex fluids. Currently, students are actively involved in the following areas:

(a) Polymer solutions: Our efforts here involve (i) the development of in-house GPU codes at the resolution of Kuhn steps and faster algorithms for Brownian dynamics simulations, (ii) studying the effects of chain model resolution on rheological predictions and (iii) development of simpler models to predict the same. Currently, all our predictions indicate marked differences in predictions with model resolution, which could not be predicted by any conventional methods.

(b) Flow of blood in artery networks: Research in this direction started with the development of a computationally simple, yet efficient, model for blood. This new model combined a recently proposed viscosity model of blood with the migration of red blood cells for flow in a conduit. It was able to predict the correct trends for both flow and concentration (of RBCs) field for various commonly occurring situations. We followed it up with a study that further elucidates the importance of such a coupled approach to solve for blood flow. Thus, it provides a new standard for non-Newtonian model of blood.

(c) Pedestrian motion: In this problem, we model human beings as “particles”, which move due to driving forces and interactions with other obstacles and other pedestrians. The “macroscopic” behaviour in various scenarios arise out of these “microscopic” interactions. Our most important contribution is a clear understanding of the role of human intelligence in the process. The long term goal is to develop a tool that enables the designing of public spaces, especially in the Indian context. In near future, we should be able to provide algorithms for self-driving segways, as well as create an extension for the flow of traffic.

Selected Publications:

1. P. Kumar, I. S. Dalal, Effects of chain resolution on the configurational and rheological predictions from Brownian dynamics simulations of an isolated polymer chain in flow, arxiv preprint arXiv:2208.04457 (2022).

2. P. Giri, K. Chandran, K. Muralidhar, I. S. Dalal, Effects of coupling of mass transport and blood viscosity models for microchannel flows, Journal of Non-Newtonian Fluid Mechanics, 302, 104754 (2022).

3. A. Goswami, I. S. Dalal, J. K. Singh, Universal Nucleation Behavior of Sheared Systems, Physical Review Letters, 126, 195702 (2021).

4. I.S. Dalal, P. Kumar, R. G. Larson, Accurate Closure for the Configuration Dynamics and Rheology of Dilute Polymer Chains in Arbitrary Flows, Macromolecules, 54, 6355 (2021).

Ishan Bajaj

Assistant Professor

PhD, Texas A&M University
Contact: Ph No: +91-512-679-2375
Email:ibajaj@iitk.ac.in
Web:https://www.iitk.ac.in/che/ishan.htm

Awards and Honours:

- Distinguished Graduate Research Award, Department of Chemical Engineering, Texas A&M University (2018)
- Finalist, CAST Directors' Student Presentation Award, AIChE (2018)
- Process Systems Engineering Young Researcher Award, CAST, AIChE (2018)

Research:

Our research group aims to develop optimization theory, models, and algorithms with applications in energy, environment, sustainability, and operations research. Our interdisciplinary research lies at the interface of chemical engineering, applied mathematics, and data science. Currently, we are working in three major areas. First, we are working on multi-scale optimization of energy and process systems to (a) optimize the design and operating conditions of the system components, (b) identify the cost-effective materials, and (c) design the supply chain network.

Second, we are developing second-order methods to optimize non-convex problems. Non-convex problems are ubiquitous in science and engineering. For instance, the loss function encountered while training neural networks is non-convex. Newton's method is a well-known second-order method that guarantees a quadratic convergence rate. However, it fails to converge when it encounters a point where the Hessian is indefinite. Accordingly, we are developing strategies to address this challenge.

Third, we are developing optimization models for the selection, design, operation, and supply chain design of electricity production, storage, and transmission technologies that can sustainably and reliably meet the growing electricity demand of India. The model accounts for the non-uniform availability of resources, spatial variation in electricity demand, and intermittency of renewable energy technologies. We are also exploring various machine learning techniques to solve the large-scale model efficiently.

Selected Publications:

1. X. Peng, I. Bajaj, M. Yao, T. W. Root, C. T. Maravelias, Solid-gas thermochemical energy storage strategies for concentrating solar power: optimization and system analysis, Energy Conversion and Management, 245, 114636 (2021).

2. H. Chang, I. Bajaj, A. H. Motagamwala, A. Somasundaram, G. W. Huber, C. T. Maravelias, J. A. Dumesic, Sustainable production of 5-hydroxymethyl furfural from glucose for process integration with high fructose corn syrup infrastructure., Green Chemistry, 23, 3277 (2021).

3. I. Bajaj, X. Peng, C. T. Maravelias, Material Screening for Thermochemical Energy Storage in Solar Power Systems, Computer Aided Chemical Engineering, 50, 179 (2021).

4. H. Chang, I. Bajaj, G. W. Huber, C. T. Maravelias, J. A. Dumesic, Catalytic strategy for conversion of fructose to organic dyes, polymers, and liquid fuels, Green Chemistry, 22, 5285 (2020).

Jayant Kumar Singh

Professor & Head

Poonam & Prabhu Goel Chair Professor
PhD, State University of New York at Buffalo
Contact: | Ph No: +91-512-259-6141
Email:jayantks@iitk.ac.in
Web:https://home.iitk.ac.in/~jayantks

Awards and Honours:

- NASI- Reliance Industries Platinum Jubilee Award (2022)
- Deepak Group's Padma Bhushan Prof. L K Doraiswamy Chemcon Distinguished Speaker Award (2022)
- Fellow, Indian National Academy of Engineering (2022)
- Herdillia Award of the Indian Institute of Chemical Engineers for excellence in basic research (2021)
- Fellow, National Academy of Science, India (2021)
- SERB - Science and Technology Award for Research (SERB-STAR) (2020)
- Mr. and Mrs. Gian Singh Bindra Chair Professor (2017-2020)
- JSPS Invitation Fellowship (2017)
- PK Kelkar (1970 Batch Fellowship), IIT Kanpur (2013-2016)
- Humboldt Research Fellowship for Experienced Researchers (2012)
- Amar Dye-Chem Award, IIChE (2010)
- INAE Young Engineer Award (2009)

Research:

My group's key focus is understanding and developing new molecules/materials for energy, environment, and health applications. We use ab-initio tools, Monte Carlo and Molecular dynamics, and Coarse-grain molecular dynamics. We also actively develop methods and tools in this area. In addition, we use machine learning and AI to accelerate the discovery of new materials and drugs.

Current thrust areas are:

- Development of materials for CO_2 capture, storage, and conversion
- Hydrogen generation and storage
- Supercooled liquid, confined fluids & nucleation
- Understanding the phase diagram of mix-surfactant systems
- Thermodynamics of Lipid-drug systems

In addition to the above, we actively work in product development. The current priority is in the area of soil health and oral cancer detection.

Selected Publications:

1. M. Bhendale, A. Srivastava, J. K. Singh, Insights into the Phase Diagram of Pluronic L64 Using Coarse-Grained Molecular Dynamics Simulations, Journal of Physical Chemistry B, 126, 4731 (2022).

2. S. H. Mir, V. K. Yadav, J. K. Singh, Efficient CO_2 capture and activation on Novel Two-Dimensional Transition Metal Borides, ACS Applied Materials & Interfaces, 14, 29703 (2022).

3. V. Parey, B. M. Abraham, S. H. Mir, J. K. Singh, High-Throughput Screening of Atomic Defects in MXenes for CO_2 Capture, Activation, and Dissociation, ACS Applied Materials & Interfaces, 13, 29703 (2022).

4. A. Goswami, I. S. Dalal, J. K. Singh, Universal Nucleation Behavior of Sheared Systems, Physical Review Letters, 126, 195702 (2021).

K. P. Krishnaraj

Assistant Professor

PhD, IISc Bangalore

Contact: | Ph No: +91-512-259-2297
Email:krishnaraj@iitk.ac.in

Web:https://www.iitk.ac.in/che/krishnaraj.htm

Awards and Honours:

- DST INSPIRE Faculty Award (2020)
- APS DFD Enabling Grant (2016)

Research:

Disordered media like granular materials are a familiar form of matter that we encounter in our daily lives, prevalent in the natural world and important in the context of geomechanics and material processing. Despite their ubiquity and significance, the mechanics of static and dense flowing granular media are complex and challenging to predict. In static and dense flowing states, the transport properties and mechanical behaviour of these forms of material are considerably influenced by the microstructure i.e., spatial arrangement of their constituents. However, the prediction and characterisation of microstructure is challenging using traditional methods and new ways are currently being explored.

We seek tools and ideas from diverse fields like complex network analysis and percolation theory that could enable us to study and characterise microstructure in a broad class of athermal disordered media like foams, dense suspensions, emulsions, and even biological cells. The knowledge gained by studying the evolution and organisation of microstructure could potentially help us develop predictive continuum models for disordered materials. Quite recently, we have developed a microstructure-based continuum model for static granular materials deposited under gravity. The model is unlike elastic, plastic or elastoplastic descriptions used by previous studies, and successfully predicts known anomalous mechanical features of static granular materials like Janssen effect in silos and central stress minimum in grain piles.

We are currently working on extending our recent model for general conditions and to develop new modelling approaches. The knowledge of microstructure in granular materials could also help us understand or uncover problems of fundamental interest. At present, we are interested in the elusive concept of “Random Close Packing” and working towards providing a comprehensive understanding of the phenomena.

Selected Publications:

1. K. P. Krishnaraj, Emergence of preferred subnetwork for correlated transport in spatial networks: On the ubiquity of force chains in dense disordered granular materials, arxiv preprint arXiv:2102.07130 (2021).

2. K. P. Krishnaraj, Spatial structure of disordered media: Unravelling the mechanical significance of disorder in granular materials, arxiv preprint arXiv:2003.02797 (2020).

3. K. P. Krishnaraj, P. R. Nott, Coherent force chains in disordered granular materials emerge from a percolation of quasilinear clusters, Physical Review Letters, 124, 198002 (2020).

4. K. P. Krishnaraj, P. R. Nott, A dilation-driven vortex flow in sheared granular materials explains a rheometric anomaly, Nature Communications, 7, 10630 (2016).

Naveen Tiwari

Professor

Raj and Neera Singh Chair Professor
PhD, University of Massachusetts
Contact: | Ph No: +91-512-679-6751
Email:naveent@iitk.ac.in
Web:https://home.iitk.ac.in/~naveent

Awards and Honours:

- Prof. Arakare Fellowship, IIT Kanpur (2020-2023)
- Young Faculty Research Award, IIT Kanpur (2020)
- Excellence in Teaching Award, IIT Kanpur (2019)
- Young Faculty Research Award, IIT Kanpur (2017)
- Young Scientist Research Award, BRNS-DAE (2014)
- Membership of the Honor Society of Phi Kappa Phi, University of Massachusetts Amherst (2007-2008)
- Travel Grant Award, University of Massachusetts Amherst (2007)

Research:

The primary focus in our group has been on the hydrodynamic instabilities in thin liquid films. Interfacial transport has significant importance in applications such as coating-flows, micro-fabrication, microfluidics, and pattern formation. For thin films, surface tension effects become essential due to the large surface-area-to-volume ratio. In our research group, the dynamics and stability of thin liquid films flowing over solid substrates are analyzed for various physical conditions on the substrate. The instability of the flow may lead to rupture of the film, which is not desired for coating applications but can be of importance for pattern formation for certain applications. In our group we investigate the effects of physical processes such as thermo-solutal Marangoni convection, long-range intermolecular interactions, evaporation at the interface, and structural heterogeneity at the solid substrate on the stability behavior of the liquid film. The mathematical models are developed starting from the usual flow and energy equations using asymptotic methods, and modal and non-modal growth of a perturbation is studied for generalized stability analysis. The equations are solved using various numerical techniques. Interesting flow patterns can be observed due to the effect of various physical processes at interplay at that length scale. Our group has also performed complete numerical simulations to study the flow of complex fluids under different configurations such as flow around a cylinder, both confined and unconfined and also flow in T-channels. We also engage with various industries in their efforts to improve and scale-up the manufacturing processes through numerical modeling.

Selected Publications:

1. G. Singh, N. Tiwari, Thin film dynamics using lattice Boltzmann method: Role of aspect ratio and surface wettability gradient, Physics of Fluids, 34, 072104 (2022).

2. D. Kishal, N. Tiwari, Role of suction pressure in the stability of a gravity-driven thermoviscous liquid film flow down the interior surface of a cylinder, European Physical Journal E, 44, 100 (2021).

3. T. C. Kumawat, N. Tiwari, Flow and stability of a gravity-driven thin film over a locally heated porous wall, Physics of Fluids, 32, 092106 (2020).

4. S. Khanum, N. Tiwari, Gravity-driven thermoviscous liquid film down a heated or cooled vertical cylinder, Physical Review Fluids, 5, 094005 (2020).

Nishith Verma

Professor

Chevron Corporation Chair Professor
PhD, University of Arizona
Contact: | Ph No: +91-512-259-6767
Email: : nishith@iitk.ac.in
Web:https://home.iitk.ac.in/che/nv.htm

Awards and Honours:

- Fulbright-Nehru Academic and Professional Excellence Fellowship (2018-2019)
- Raj and Neera Singh Chair, IIT Kanpur (2015-18)
- Fellow, Royal Society of Chemistry, UK (2015)
- Raj and Neera Singh Chair, IIT Kanpur (2011-14)
- Alexander von Humboldt Research Fellow (2004)
- AICTE career award for young teachers (1998)
- S. K. Nandi Memorial Merit Scholarship, IIT Kharagpur (1985-86)

Research:

Our research laboratory continues to synthesize novel materials to address energy, environmental, and health aspects of chemical engineering. In particular, our research themes focus on the development of carbon-based materials, viz. carbon nanofibers in the adsorption and catalytic reaction engineering applications including microbial fuel cells for wastewater treatment; microbial electrolysis systems for generating different value-added products via the electrochemical reduction of CO_2; photocatalysis; electrochemical hydrogen generation, and membrane separation. In the area of chemical engineering processing, new methods are being explored. These include advanced oxidation processes including catalytic wet air oxidation for the treatment of industrial aqueous effluents containing high organic loadings. Another study is underway to develop chemical and biosensors using metal-polymer-carbon-based composite materials. The route for developing such sensors is novel, using the principles of electrochemistry and chemiresistivity. On the theoretical side, a number of mathematical models based on lattice Boltzmann method have been developed to predict the breakthrough curves in the narrow tubular packed bed adsorber. Over the years, these studies have resulted in several national and international patents that include a system for simultaneous detection of cholesterol, creatinine and glucose; carbon fibers for removing soil toxic metals and increasing micronutrient supply to plants, and the development of micronutrients with the new formulation of M-CNF. Most notably, the joint collaboration between IIT Kanpur and Shell International Research Maatschappiz BV, The Netherlands, has resulted in three joint USA patents granted, covering a method for preparing the catalytic carbon beads to treat the high COD (~125,000 mg/L) containing wastewater effluents released by the styrene manufacturing petrochemical plants, using advanced oxidation process. Many of these studies and research activities are being supported through the sponsored and consultancy projects, involving graduate as well undergraduate students, and project research staff.

Selected Publications:

1. P. Gupta, N. Verma, Conversion of CO_2 to Formate using Activated Carbon Fiber-supported g-C_3N_4-$NiCoWO_4$ Photoanode in a Microbial Electrosynthesis System, Chemical Engineering Journal, 446, 137 (2022).

2. J. K. George, N. Verma, Super-hydrophobic/Super-oleophilic carbon nanofiber-embedded resorcinol-formaldehyde composite membrane for effective separation of water-in-oil emulsion, Journal of Membrane Science, 654, 15 (2022).

3. H. Ali, N. Verma, A Hybrid UV-Vis Spectroelectrochemical Approach for Measuring Folic Acid using a Novel Ni-CNF/ITO Electrode, Electrochimica Acta, 428, 140920 (2022).

Nitin Kaistha

Professor

PhD, University of Tennessee
Contact: Ph No: +91-512-259-7513
Email:nkaistha@iitk.ac.in
Web:https://home.iitk.ac.in/~nkaistha

Awards and Honours:

- Chevron Corporation Chair Professor, IIT Kanpur (2018-2021)
- Visiting Chemical Engineering Faculty, Nanyang Technical University (NTU), Singapore (2012-14)
- PK Kelkar Outstanding Young Researcher Fellowship, IIT Kanpur (2009-12)
- Erasmus Mundus External Cooperation Window Lot 13 Fellowship at Norwegian University of Science and Technology (NTNU), Norway (2009)

Research:

Our research focuses on process integration for improved material and energy utilization efficiency and its implications on plant design, operation and control. The integration makes the design of a robust plantwide control to reduce the overdesign for a controllable plant system particularly challenging due to the high non-linearity and multiway dynamic interaction introduced by the material and energy recycle loops. Our research has made significant contributions towards developing a systematic procedure for addressing fundamental plantwide control system design questions of what process variables to control for satisfying the safety, stability and economic objectives, and synthesizing a robust control structure (pairing with control inputs and other enhancements) for controlling the same. We are also researching the systematic leveraging of the immense flexibility in plantwide control system synthesis to optimize the process design for controllability.

Selected Publications:

1. N. Kaistha, Liquid level control in a recycle loop, Journal of Process Control, 104, 11 (2021).
2. V. Kumar, N. Kaistha, Design and Control of a Vapour Recompression C3 Splitter, Chemical Engineering Research and Design, 159, 410 (2020).
3. V. Kumar, N. Kaistha, Inferential self-optimizing control of a reactor-separator-recycle process, Industrial & Engineering Chemistry Research, 58, 15209 (2019).
4. V. Kumar, N. Kaistha, Invariants for optimal operation of a reactor-separator-recycle process, Journal of Process Control, 82, 1 (2019).
5. V. Kumar, N. Kaistha, Real-Time optimization of a reactor–Separator–Recycle process II: dynamic evaluation, Industrial & Engineering Chemistry Research, 58, 1966 (2019).
6. K. Mishra, N. Kaistha, Synthesis, design, and control of an azeotropic distillation system for methanol–isopropyl acetate separation, Industrial & Engineering Chemistry Research, 58, 1229 (2018).
7. V. Kumar, N. Kaistha, Real Time Optimization of a Reactor–Separator–Recycle Process I: Steady State Modeling, Industrial & Engineering Chemistry Research, 57, 12429 (2018).

Pankaj A. Apte

Associate Professor

PhD, Ohio State University
Contact: | Ph No: +91-512-259-7459
Email:papte@iitk.ac.in
Web:https://home.iitk.ac.in/~papte

Awards and Honours:

- Outstanding graduate student award for academic achievement, Ohio State University (2006)
- Gold Medal, B.Tech., Nagpur University (1998)

Research:

Current research in my group is focussed on exploring the cooperative phenomena in phase transitions. When cooperativity is established, atoms or molecules in the whole system act concertedly such that the system, it its entirety, is driven in a specific direction leading to a transition. Many of the phase transitions remain poorly understood due to lack of recognition of the underlying cooperative phenomena. Recently we have shown that ordering transition in Ni_3Fe alloy is caused by cooperative freezing of the L12 ordered domains at the critical temperature and the resulting propagation of the domains upon further cooling. A practical manifestation of this cooperative freezing is the critical slowing down, i.e., a significant increase in equilibration time (to 40 days or more) during annealing of Ni_3Fe alloy as the critical temperature (500 °C) is approached. Another important class of transitions are those responsible for formation of tetrahedral amorphous materials. We found that cooperative relaxation of the tetrahedral network transforms supercooled water into stacking disordered ice, also known as low density amorphous (or LDA) ice. A similar transition is also found in supercooled silicon that leads to formation of amorphous silicon which is commonly used in solar cells. A related research activity in my group is the investigation of structural changes in tetrahedral materials based on ring based mesostructures. We have proposed and implemented a method to identify the rings with specific shapes using puckering method which was originally developed (about five decades ago) to analyse organic ring compounds. With this method, we have been able to identify the boat and chair shaped six-membered rings. Such rings form the basis of mesostructures that are commonly found in tetrahedral materials. Using this approach, we have introduced a new method to identity hexagonal crystalline particles in amorphous materials. We have also explored ring based defect structures such as pentagonal nanochannels which, potentially, have a profound influence on the bulk properties of amorphous ice. Apart from these theoretical and computational approaches, we have also recently started experimental work to understand ionic equilibria in problems of practical interest. In particular, we are working on CO_2 absorption in aqueous potassium carbonate solutions with small amounts of added promoters. Such absorption processes are commonly employed in fertilizer industry. Our aim is to understand the ionic equilibria responsible for enhancement of absorption rates due to added promoters such as diethanol amine and glycine. In collaboration with the heterogeneous catalysis group (Prof. Goutam Deo), we are also investigating the use of Alumina supported Ni_3Fe as a catalyst for CO_2 methanation reaction.

Selected Publications:

1. Anil Mangla, Goutam Deo, Pankaj A. Apte, Cooperative freezing of the L12 ordered domains at the critical cooling temperature of Ni_3Fe alloy, Journal of Statistical Mechanics : Theory and Experiment, 2022, 093204 (2022).

2. Nandlal Pingua, Pankaj A. Apte, Topological Identification Criteria, Stability, and Relevance of Pentagonal Nanochannels in Amorphous Ice, Journal of Physical Chemistry B, 123, 10301 (2019).

Raghavendra Ragipani

Assistant Professor

PhD, IIT Bombay & Monash University

Contact: | Ph No: +91-512-259-2241
Email:ragipani@iitk.ac.in
Web:https://home.iitk.ac.in/~ragipani

Awards and Honours:

- Naik and Rastogi Excellence in Ph.D. Thesis Award, IIT Bombay (2021)

Research:

My research is focused on process intensification and sustainable process development. One of the key areas is carbon dioxide capture, including direct air capture (DAC) and its mineralisation to stable carbonates using alkaline industrial wastes such as coal ash and steel slags. The problem of solid waste utilisation is an equally pertinent question to today's rapidly growing consumption-driven society. We work on integrated DAC-mineralisation processes and product development to address CO_2 removal and solid waste use simultaneously. Catalytic conversion of CO_2 into chemicals is also an area of interest.

Another area of research interest is to develop surrogate models and digital twins using machine learning (ML). Our research focuses on developing Physics Informed Neural Networks (PINN). We are also looking at the paradigm of developing autonomous modular reactors, wherein process control and real-time optimisation are achieved using AI-ML models. At a fundamental level, we are interested in modelling and analytical solutions for reactive surface area evolution in heterogeneous fluid-solid reactions, the role of surface electrical properties at the solid-liquid interface, and novel high-throughput experiment designs and analyses.

Selected Publications:

1. Raghavendra Ragipani, Direct Air Capture and Sequestration of CO_2 by Accelerated Indirect Aqueous Mineral Carbonation under Ambient Conditions, ACS Sustainable Chemistry & Engineering, 10, 7852 (2022).
2. Raghavendra Ragipani, Sankar Bhattacharya, Akkihebbal K. Suresh, A review on steel slags valorisation via mineral carbonation, Reaction Chemistry & Engineering, 6, 1152 (2021).
3. Raghavendra Ragipani, Kinetics of steel slag dissolution: from experiments to modelling, Proceedings of the Royal Society A, 475, 20180830 (2019).
4. Raghavendra Ragipani, Towards efficient calcium extraction from steel slag and carbon dioxide utilisation via pressure-swing mineral carbonation, Reaction Chemistry & Engineering, 4, 52 (2019).

Raghvendra Singh

Associate Professor

PhD, State University of New York at Buffalo

Contact: | Ph No: +91-512-259-7605
Email:raghvend@iitk.ac.in

Web:https://home.iitk.ac.in/~raghvend

Awards and Honours:

- Chemical engineering graduate student fellowship, State university of New York at Buffalo (2001-2005)
- Biomedical Engineering Society (BMES) Travel Award (2004)
- New York State-GSEU Professional Development Award (2003)

Research:

Stem cells are at the core of the normal developmental processes and in many pathological conditions. We study both embryonic and adult stem cell fate decisions using systems biology approach in the context of both normal homeostasis and in human diseases. Further, stem cell fate decisions are stochastic in nature. We apply statistical mechanics to study the lineage and differentiation of these cells.

Selected Publications:

1. Alok Jaiswal, Raghvendra Singh, Homeostases of epidermis and hair follicle, and development of basal cell carcinoma, Biochimica et Biophysica Acta (BBA) - Reviews on Cancer, 1877, 188795 (2022).

2. Raghvendra Singh, Basal cells in the epidermis and epidermal differentiation, Stem cell Reviews and Reports, 18, 1883 (2022).

3. S. Gupta, Raghvendra Singh, Analysis of the Virus Dynamics Model Reveals That Early Treatment of HCV Infection May Lead to the Sustained Virological Response, PLoS ONE, 7, e41209 (2012).

Rahul Mangal

Associate Professor

PhD, Cornell University
Contact: Ph No: +91-512-679-2002
Email:mangalr@iitk.ac.in
Web:https://home.iitk.ac.in/~mangalr

Awards and Honours:

- Class of 1979, Young faculty fellowship, IIT Kanpur (2021-2024)
- Young Engineer Award, Indian National Academy of Engineering (2020)
- Ramanujan Fellowship, SERB (2017)
- Early Career Research Award, SERB (2019)

Research:

My research group is currently investigating various fundamental aspects of Active Soft matter and Polymer Composites. Active soft-matter systems are capable of extracting energy from their surroundings to perform the out-of-equilibrium mechanical motion and they have been postulated to be capable of performing intricate tasks in microscopic domains such as drug delivery, bio-sensing, isolation of pathogens, environmental remediation, micromachines, etc. These lifeless synthetic motors can also mimic the locomotion of several biological micro-swimmers, including common pathogens such as bacteria, and provide useful insights into their response to external stimuli. In recent years, my group has explored the effect of external shear flow, chemical additives, and passive tracers, on the motion of both artificial active Janus particles and active droplets, in Newtonian surroundings. Lately, I have also started to explore the dynamics and self-assembly characteristics of artificial swimmers in non-Newtonian surroundings. In near future, through our carefully designed experiments, I aim to contribute significantly to the advancement of the overall fundamental understanding of artificial swimmers in complex fluids.

My group has also been working on developing polymer adhesive films with surface and sub-surface patterning for which the design principles are borrowed from living creatures such as geckos, mussels, tree frogs, octopuses, etc. We recently fabricated a porous adhesive film with a thin viscoelastic layer on top which not only provided better adhesion but also better absorption of impact shock. The design principles of tree frogs and mussels were combined to achieve enhanced properties. Through this work in our group, we have produced two research articles. The long-term objective is to design novel smart robust adhesives for health care applications. In the latter, carefully designed nanocomposite materials are exposed to controlled shockwaves generated in shock tubes at Mach number ~ 1.6. The effect of shockwaves on the material strength and structure is investigated through imaging and bulk rheology measurements. Results from these experiments will lay the foundation for the synthesis of composites capable to offer maximum resistance against shock waves which can be very useful in defense applications.

Selected Publications:

1. P. Dwivedi, A. Shrivastava, D. Pillai and R. Mangal, Deforming Active Droplets in Viscoelastic fluid , https://arxiv.org/abs/2209, 14348 (2022).

2. P. Dwivedi, A. Shrivastava, D. Pillai and R. Mangal, Rheotaxis of Active Droplets, Physics of Fluids, 33, 082108 (2022).

3. P. Dwivedi, B. R. Si, D. Pillai and R. Mangal, Solute Induced Jittery Motion in Active Droplets, Physics of Fluids, 33, 022103 (2021).

Raj Ganesh S Pala

Professor

PhD, University of Utah
Contact: Ph No: +91-919-826-1694
Email:rpala@iitk.ac.in
Web:https://home.iitk.ac.in/~rpala

Awards and Honours:

- Indian Oil Golden Jubilee Professorial Chair Professor, IIT Kanpur (2019-2022)

Research:

Raj Ganesh Pala leads the Electrochemical, Catalytic and Separations Engineering Laboratory ("ECCSEL"), which is composed of personnel with a blend of experimental and computational skills not only in chemical science and engineering but also in mechanical and instrumentation engineering. Raj strongly believes in an interdisciplinary approach to engineering research and product development. An important theme of Raj's electrochemical research is Solar Hydrogen as a "renewable reductant," wherein Hydrogen is generated from a renewable feed (like water) and renewable energy. The ultimate goal of this effort is to electrochemically sequester the so generated Hydrogen with Carbon dioxide to produce hydrocarbons relevant to the chemical industry. In the near term, hydrogen cogeneration with value-added chemicals like Chlorine, Potassium Chlorate, pure Oxygen, and Hydrogen generating water electrolyzer driven via solar photovoltaic is being attempted. In addition to these areas, the group also explores material design for Lithium Ion Batteries, electrochemical taste sensors and fundamental aspects of electrochemical impedance spectroscopy.

A long-standing interest of Raj's group has been to design "non-native" nanostructures and demonstrate their utility in material-centric energy conversion and storage devices. Non-native and energetically ground state "native" structures differ in their discrete translational crystal symmetry. Raj's group has proposed that coupling molecular events in the material device gives rise to contra-varying or co-varying properties that provide bounds on efficiency. Heterostructures have been rationally designed and demonstrated via non-native structures to decouple molecular events that limit efficiency in cathodes of Lithium Ion Batteries, Photo-electrochemical-anodes, and a variety of electrocatalysts.

A recent thrust is explorations in magneto-electrochemical systems (to promote oxygen evolution electrocatalysis) and in physicochemical phenomena (like nuclear transmutation, carbon nanotube generation, and localized plasma generation) via very high voltage electrochemical systems.

Selected Publications:

1. A. K. Ummireddi, S. K. Sharma, Raj Ganesh S. Pala., Tetraethylammonium Cation Tuned Electrochemical CO_2 Reduction and Hydrogen Evolution Reaction Activities on Transition Metals (Cu, Ag, Ni, and Fe), Journal of Catalysis, 406, 213 (2022).

2. S. Saha, K. Kishor, Raj Ganesh S. Pala, Climbing up the volcano through support-electrocatalyst interaction in electrodeposited thin metal oxides for oxygen evolution reactions, Catalyst Science Technology, 11, 4342 (2021).

3. P. K. Gupta, A. Bhandari, J. Bhattacharya, Raj Ganesh S. Pala, Higher Voltage, Wider Voltage Plateau, Longer Cycle Life, and Faster Kinetics via Thermally Modulated Intergrowth Structure of Ramsdellite and Pyrolusite MnO2 for Lithium-Ion Battery Cathodes, Journal of Power Sources, 450, 227619 (2020).

Raju Kumar Gupta

Professor

PhD, National University of Singapore

Contact: | Ph No: +91-512-259-6972
Email:guptark@iitk.ac.in
Web:https://home.iitk.ac.in/~guptark

Awards and Honours:

- P.K. Kelkar Young Faculty Fellowship, IIT Kanpur (2022-2025)
- Distinguished Young Alumnus Awards (DYAA), IIT Roorkee (2021)
- P. K. Kelkar Young Faculty Research Fellowship, IIT Kanpur (2018)
- Young Scientist Award, Council of Science & Technology, Uttar Pradesh, India (2014-15)
- IEI Young Engineer Award in engineering discipline by The Institution of Engineers, India (2014-15)
- INSPIRE (Innovation in science pursuit and inspired research) faculty fellowship by Indian National Science academy (INSA) and Department of Science and Technology (DST), India (2013-2018)

Research: Our research group at IIT Kanpur focuses on the development of nanostructured materials for energy and environmental applications. Our research interests include green synthesis, photocatalysis for water remediation and conversion of CO_2 to fuels, hybrid perovskite solar cells and energy storage devices. We have done considerable work in the area of photocatalysis for water remediation, hybrid perovskite solar cells, high dielectric constant materials and supercapacitors. Key highlights of our research works are given below:

(a) Noble photocatalytic systems for degradation of pollutants towards wastewater treatment applications- Our group has developed various nanostructured photocatalysts, improved their photocatalytic activity for degradation of organic compounds via enhancement in visible light absorption as well as in charge separation at the interface and further, immobilized these photocatalysts over flexible support to prevent their elution in streamflow leading to their usage in a reactor system.

(b) Interface engineering towards improved performance of perovskite solar cells- Our group has focused on understanding film formation of the perovskite materials and composition/interface engineering for perovskite solar cells (PSCs). The low electrical conductivity of TiO_2 is an obstacle to PSC efficiency enhancement. We have studied the conductivity enhancement of TiO_2 by tantalum (Ta) doping and its effect on improving the device performance. We have also incorporated PC70BM as an additive in the perovskite layer. This led to the formation of larger grains with fewer grain boundaries and reduced charge carriers recombination. The devices using PC70BM additive exhibited over 15% improvement in the power conversion efficiency.

(c) Development of metal oxide/polymer nanocomposites for energy storage devices applications- Our group has majorly focussed on the development of energy storage devices e.g. supercapacitors and capacitors. We have developed non-aggregated polymeric/ceramic hybrid materials for capacitor-based devices and nanostructured materials for supercapacitor applications. The overall objective is to synergistically enhance energy storage performance in terms of both the energy and power density via structural engineering and careful selection of materials.

Selected Publications:

1. Prateek, R. Bhunia, S. Gupta, A. Garg, R. K. Gupta, In-situ fabrication of $BaTiO_3$@PVP in PVDF polymer nanocomposites for dielectric capacitor applications, Journal of Polymer Science, 60, 961 (2022).

2. P. Kar, K. Shukla, P. Jain, R. K. Gupta, Activated Carbon Fiber Supported Fe_2O_3@Bismuth Carbonate Heterojunction for Enhanced Visible Light Degradation of Emerging Pharmaceutical Pollutant, Reaction Chemistry & Engineering, 6, 2029 (2021).

Sanjeev Garg
Professor

PhD, University of Connecticut
Contact: Ph No: +91-512-259-7736
Email:sgarg@iitk.ac.in
Web:https://home.iitk.ac.in/~sgarg

Research:

The recent research activity in the Computer Aided Product and Process Design Laboratory are focussed on Health and Environmental applications using Molecular Biology and Mathematical Programming. A few of the ongoing project activities are mentioned below.

The aim of one of the projects in our research group is to evaluate small interfering RNAs (siRNA) as a therapeutic for the Alzheimer's disease (AD) using in silico and in vitro frameworks. RNA interference (RNAi) with siRNAs is a powerful tool to down regulate the genetic flow at transcriptional level. Different empirical and rational design criteria are being evaluated for siRNA mediated BACE1 gene silencing in murine neuronal cell lines. This project also focuses on the delivery of siRNAs selected from the in vitro verified and in silico designed siRNAs. The project aims to provide a comparison of siRNA delivery and silencing using different gold nanoparticle layer-by-layer nano-assemblies (AuNP LbL NAs) in neuronal cell lines for BACE1 gene silencing. The uptake mechanism is also being evaluated using chemical inhibition of the endocytosis pathways. Preliminary results conclude that the AuNP LbL NA primarily follow macropinocytosis for cellular entry.

The major aim of another project is to develop a novel wastewater treatment technology using recombinant bacteria for source point application. Sulphonated azo dyes are used in various industries and are known to be xenobiotic and highly carcinogenic and mutagenic to humans. Various physicochemical methods for azo dye degradation are not environment friendly and hence the bioremediation of azo dyes is gaining research momentum. The biological treatment methods developed in the last few decades are proven to be efficient. In our group, azoreductase gene, azoK, (encoding for azo dye degrading enzyme, azoreductase) from the isolated Klebsiella pneumoniae (a pathogenic strain that cannot be used directly in the process) is cloned and heterologously expressed in E. coli. The viability of the recombinant azoK for bioremediation of the azo dyes from industrial wastewater is established. Work is ongoing to clone protoK in E. Coli to carry out the conversion of aromatic amines (metabolites produced during aromatic dye degradation) to nontoxic smaller compounds. This project intends to develop a novel bioremediation process for source point application in near future. Another project activity is aimed at rationally designing diffusion-controlled drug delivery devices for the controlled release of an anticancer drug, Paclitaxel, using in silico mathematical models in a reverse engineering framework. Specifically, semi-empirical QSPR models for mutual diffusion coefficients of the drug in biocompatible and biodegradable polymers and the partition coefficients of the drug between polymers and blood are being developed.

Selected Publications:

1. S. Dixit, S. Garg, Enzymatic degradation of sulphonated azo dye using purified azoreductase from facultative Klebsiella pneumoniae, Folia Microbiologica, 66, 79 (2020).

2. A. Pramanik, S. Garg, Design of diffusion-controlled drug delivery devices for controlled release of Paclitaxel, Chemical Biology & Drug Design, 94,1478 (2019).

3. P. Chaudhari, S. Garg, Multi-Objective Optimization of Maleic Anhydride Circulating Fluidized Bed (CFB) Reactors, Chemical Engineering Research and Design, 141, 115 (2019).

Siddhartha Panda

Professor

Dr. S. Sampath Chair Professor
PhD, University of Houston
Contact: Ph No: +91-512-259-2040
Email:spanda@iitk.ac.in
Web:https://home.iitk.ac.in/~spanda

Awards and Honours:

- Golden Jubilee Chair Professor on Entrepreneurship and Innovation, IIT Kanpur (2018-2021)
- Jeet Bindra Research Fellowship (2010-2013)
- IBM Invention Achievement Award (2002-2006)

Research:

Our research activities are in the areas of transport phenomena, reaction engineering, materials processing and micro/nano fabrication leading to the technology development of physical and chemical sensing elements (electrochemical, chemiresistive, thin film transistors based) - utilizing both printable flexible electronics based platforms as well as conventional silicon electronics based platforms. We study the physical modifications and chemical modifications to fabricate functional sensing surfaces, transport phenomena of the analytes to these surfaces (including in microfluidic units), the specific recognition reactions at these surfaces, charge transport in the semiconducting materials, and device design (including arrays). There is an effort towards understanding the sensing mechanisms. There are activities on developing the systems to utilize these sensing elements and add “smartness” to these systems. These are utilized in-vitro diagnostic devices and flexible wearable systems in healthcare applications, food quality monitoring, and assistive technologies.

Selected Publications:

1. S. Verma, S. Panda, Study of capture efficiency utilizing passive mixing in heterogeneous microfluidic immunosensors, Chemical Engineering and Processing –Process Intensification, 180, 108708 (2022).

2. S. K. Gautam, N. A . Gokhale, S. Panda, Mechanism of NH_3 gas sensing by SnO_2/PANI nanocomposites: charge transport and temperature dependence study, Flexible and Printed Electronics, 7, 035022 (2022).

3. M. Sinha, M. K. Rana, S. Panda, Templated growth of polyaniline for enhanced gas sensing response in flexible sensors: experiments and simulations, Flexible and Printed Electronics, 6, 035007 (2021).

4. A. N. Mallya, S. Panda, DFT study of iminodiacetic acid functionalised polyaniline copolymer interaction with heavy metal ions through binding energy, stability constant and charge transfer calculations, Computational and Theoretical Chemistry, 1202, 113288 (2021).

5. S. K. Gautam, S. Panda, Effect of moisture and molecular weight of polyaniline on H_2S sensing characteristics, Sensors and Actuators B: Chemical, 344, 130323 (2021).

6. V. S. Rathaur, S. Kumar, P. K. Panigrahi, S. Panda, Investigating the effect of antibody-antigen reactions on the internal convection in a sessile droplet via micro particle image velocimetry and DLVO analysis, Langmuir, 36, 8826 (2020).

Soumik Das

Assistant Professor

PhD, University of Texas at Austin

Contact: Ph No: +91-512-679-2385
Email: dsoumik@iitk.ac.in

Web: https://www.iitk.ac.in/che/sdas.html

Awards and Honours:

- Thomas H. and Dorothy M. Timmins Endowed Graduate Fellowship (UT Austin 2019-20)
- Cockrell School of Engineering Fellowship (UT Austin 2018-19)
- Professional Development Award (UT Austin 2016-18)
- George J. Heuer, Jr. Ph.D. Endowed Graduate Fellowship (UT Austin 2014-15)

Research:

Recent years have witnessed a tremendous surge in the use of composite materials across multiple research communities. Composites, which involve an innovative combination of different materials, enable synergistic enhancement of the properties of individual components. For example, nanoparticle-hydrogel composites can exhibit superior mechanical properties compared to the hydrogel itself, and at the same time improve the stability of the nanoparticles against aggregation. Exciting strategies involving a rational selection of hybrid or composite materials to modulate interfaces have further opened new directions in the field of materials discovery with unique bulk and interfacial properties. In our group, we plan to harness the plurality of bulk and interfacial properties offered by organic-inorganic composites to fabricate functional materials, with potential applications in green enhanced oil recovery (EOR), carbon capture, programmable and multi-responsive emulsions, and atmospheric water harvesting (AWH).

A second aspect of the research in our group would be to use structured solvents like liquid crystals as templates for molecular assembly and synthesis of functional materials. The central theme in this direction would be to translate the anisotropic order of these solvents into well-defined hierarchical structures that possess macroscale anisotropy. Such structures are quite prevalent in many biological systems and have potential applications in membrane separations, nanofluidic osmotic energy conversion and energy storage devices.

Selected Publications:

1. Soumik Das, JungHyun Noh, Wei Cao, Hao Sun, Nathan C Gianneschi, Nicholas L Abbott, Using Nanoscopic Solvent Defects for the Spatial and Temporal Manipulation of Single Assemblies of Molecules, Nano letters, 22, 18 (2022).

2. Soumik Das, Sangchul Roh, Noe Atzin, Ali Mozaffari, Xingzhou Tang, Juan J de Pablo, Nicholas L Abbott, Programming Solitons in Liquid Crystals Using Surface Chemistry, Langmuir, 38, 11 (2022).

3. Jaehyung Yu, Ce Liang, Myungjae Lee, Soumik Das, Andrew Ye, Fauzia Mujid, Preeti K Poddar, Baorui Cheng, Nicholas L Abbott, Jiwoong Park, Two-Dimensional Mechanics of Atomically Thin Solids on Water, Nano letters, 22, 17 (2022).

4. Soumik Das, Amit Katiyar, Neeraj Rohilla, Quoc P Nguyen, Roger T Bonnecaze, Wettability alteration and adsorption of mixed nonionic and anionic surfactants on carbonates, Langmuir, 36, 50 (2020).

Sri Sivakumar

Professor

PhD, University of Victoria
Contact: Ph No: +91-512-259-7697
Email: srisiva@iitk.ac.in
Web: https://www.iitk.ac.in/che/faculty/srisiva/index.htm

Awards and Honours:

- Raj and Neera Singh Chair Professor, IIT Kanpur (2019-2022)
- Prof. CNR award for outstanding research contribution (2014)
- Class of 1979 Research Fellowship, IIT Kanpur (2013-2016)

Research:

Prof. Sri Sivakumar's group focuses on the design and development of nanomaterials for biological, catalytic and energy applications. Recently, we developed an artificial skin model using plant leaf as the scaffold. Further, we also developed a paper-based sensing device using saliva as the biofluid for oral cancer detection. Major areas of research that we undertake are:

- Stabilization and growth mechanism of nanoparticles
- Preparing catalysts for different potential fields including HDS (hydro-desulfurization) of petroleum products, fuel cell applications and oxidation reactions.
- Nanocontrast agents and drug delivery vehicles
- Solid state lighting applications
- Hydrogen production by splitting water using photo-electrochemical cell
- Photonic Crystals for low threshold lasers, optical filters, multifrequency optical Bragg Filter, Electrodes in Solar Cells etc.

Selected Publications:

1. G. P. Sharma, P. K. Gupta, S. K. Sharma, R. G. S. Pala, S. Sivakumar, Chalcogenide Dopant-Induced Lattice Expansion in Cobalt Vanadium Oxide Nanosheets for Enhanced Supercapacitor Performance, ACS Applied Energy Materials, 4, 4758 (2021).

2. C. Rajalekshmi Dhanya, J. Jeyaraman, S. Sainulabdeen, M. S. Soumya, A. Abraham, S. Sivakumar, Biocompatible Multifunctional Theranostic Nanoprobe for Imaging and Chemotherapy in Solid Tumor Bearing Mice, ChemPhotoChem, 5, 106 (2021).

3. R. Singh, D. Kunzru, S. Sivakumar, Monodispersed ultrasmall NiMo metal oxide nanoclusters as hydrodesulfurization catalyst, Applied Catalysis B: Environmental, 185, 163 (2016).

4. J. Jeyaraman, A. Shukla, S. Sivakumar, Targeted Stealth Polymer Capsules Encapsulating Ln^{3+}-Doped $LaVO_4$ Nanoparticles for Bioimaging Applications, ACS Biomaterials Science & Engineering, 2, 1330 (2016).

5. A. Rammohan, G. Mishra, B. Mahaling, L. Tayal, A. Mukhopadhyay, S. Gambhir, A. Sharma, S. Sivakumar, PEGylated Carbon Nanocapsule: A Universal Reactor and Carrier for In Vivo Delivery of Hydrophobic and Hydrophilic Nanoparticles, ACS Applied Materials & Interfaces, 8, 350 (2015).

Vishal Agarwal

Associate Professor

PhD, University of Massachusetts Amherst

Contact: | Ph No: +91-512-259-6895
Email: vagarwal@iitk.ac.in

Web:https://home.iitk.ac.in/~vagarwal

Awards and Honours:

- Ramanujan Fellowship (2017)
- RG Madhudhane M. Tech. Best Masters Research Thesis Award, IIT Bombay (2006)

Research:

The primary focus of my research group is to develop molecular-level understanding of complex systems in the areas of catalysis, biomass conversion, CO_2 conversion to fuels, H_2 generation; with the ultimate aim of assisting in better design of such processes. We use ab initio quantum chemical, molecular dynamics, monte carlo and rare-event methods to investigate the atomic features that govern the molecular transformations in these processes. We are also developing methods for efficient exploration of potential energy surfaces.

Selected Publications:

1. A. Lal Bose, V. Agarwal, Oxygen Healing and CO_2 /H_2 /Anisole Dissociation on Reduced Molybdenum Oxide Surfaces Studied by Density Functional Theory, ChemPhysChem: e202200510(2022).

2. S. K. Dutta, S. Ghosh, H. Metiu, V. Agarwal, Nascent Decomposition Pathways of CH_4 Pyrolysis in Gas Phase Metal Halides, Journal of Physical Chemistry A, 126, 5900 (2022).

3. S. K. Dutta, V. Agarwal, DFT study of phenol alkylation with propylene on H-BEA in the absence and presence of water, Reaction Chemistry & Engineering, 6, 2315 (2021).

4. R. Saxena, VBKSPK Avanigadda, R. Singh, V. Agarwal, Ab initio dynamics of gas-phase and aqueous-phase hydrolysis of adenosine triphosphate, International Journal of Quantum Chemistry, 121, e26615 (2021).

5. V. Agarwal, H. Metiu, Rates of adsorption and desorption: Entropic contributions and errors due to mean-field approximations, Journal of Chemical Physics, 150, 184702 (2019).

6. D. C. Upham, V. Agarwal, A. Khechfe, Z. R. Snodgrass, M. J. Gordon, H. Metiu, E. W. McFarland, Catalytic molten metals for the direct conversion of methane to hydrogen and separable carbon, Science, 358, 917 (2017).

7. V. Agarwal, H. Metiu, Oxygen Vacancy Formation on α-MoO_3 Slabs and Ribbons, The Journal of Physical Chemistry C, 120, 19252 (2016).

Viswanathan Shankar

Professor

Mr. & Mrs. Gian Singh Bindra-
Chair Professor
PhD, IISc Bangalore
Contact: Ph No: +91-512-259-7377
Email: vshankar@iitk.ac.in
Web:https://home.iitk.ac.in/~vshankar

Awards and Honours:

- Fellow, Indian National Academy of Engineering (2021)
- Excellence in Teaching Award, IIT Kanpur (2020)
- Distinguished Teacher Award, IIT Kanpur (2018)
- Sajani Kumar Roy Memorial Chair Professor, IIT Kanpur (2015-2018)

Research:

Our group carries out research on a range of problems of relevance to microscale flows and complex fluids (like polymer solutions and melts) with particular focus on how laminar flows become unstable, and how the rheological nature of the complex fluid affects the instabilities. We use a combination of analytical theory, computations and experiments to uncover and understand new phenoemena in these problems. One major bottleneck in the development of microfluidic technologies is the requirement of rapid rates of transport of passive scalars like heat or mass, which is generally not feasible in microscale flows owing to their small dimensions. When the channel dimensions are in the range of tens of microns, the flow regime in such devices is often laminar, and hence mixing of passive scalars in direction normal to the streamlines is limited by molecular diffusion, often a very slow process. In conventional engineering applications, this limitation is often overcome by operating the flow in the turbulent regime, where the rates of transfer are often larger by orders of magnitude due to rapid transport by turbulent eddies. However, reaching turbulent flow in rigid tubes and channels implies that the flow must operate at a Reynolds number of 2000 or more. Achieving such a large Reynolds number is very difficult in microfluidic devices due to their small dimensions. Can we achieve transition at Reynolds numbers much lower than 2000? Research carreied out in our group has shown that it is possible to achieve this, by either making the rigid wall deformable or `soft' or by altering the rheology of the fluid. What is the consequence of complex rheology on more realistic flows? In particular, what is the consequence of rheology on the laminar-turbulent transition? The research carried out in our group has shown that the deformable nature of the wall can induce instabilities in a Newtonian fluid which are absent in rigid tubes and channels, and interestingly, these instabilities happen at Reynolds numbers much lower than 2000.

In the recent years, research in Prof. Shankar's group has focused on the fundamental understanding and quantitative description of the onset of turbulence in the flow of polymer solutions and in flow through conduits with deformable walls. While the phenomenon of turbulence onset in Newtonian pipe flows is well known since the iconic experiments of Osborne Reynolds, a quantitative description of the transition is notoriously difficult owing to the flow being stable to small perturbations.

Selected Publications:

1. V. Shankar et al., Perspectives on viscoelastic flow instabilities and elastic turbulence, Physical Review Fluids, 7, 080701 (2022).

2. V. Shankar et al., Understanding viscoelastic flow instabilities: Oldroyd-B and beyond, Journal of non-Newtonian Fluid Mechanics, 301, 104742 (2022).

Yogesh M. Joshi

Professor

Pandit Girish Ranjan & Sushma Rani Pathak-Chair Professor
PhD, IIT-Bombay & NCL, Pune
Contact: Ph No: +91-512-259-7993
Email: joshi@iitk.ac.in
Web:https://home.iitk.ac.in/~joshi

Awards and Honours:

- Fellow, Indian Academy of Sciences (2023)
- Fellow, Indian National Science Academy (2022)
- Fellow of the Society of Rheology, US (SoR) (2022)
- Academy excellence award of the Defense Research and Development Organization (2019)
- Distinguished Teacher Award of IIT Kanpur (2018)
- Fellow, National Academy of Sciences, India (2017)
- Fellow, Indian National Academy Engineering (2016)
- Prof. C.V.Seshadri Chair Professor, IIT Kanpur (2015-2018)
- Shanti Swarup Bhatnagar Award in Engineering Sciences (2015)
- P.K. Kelkar Fellowship, IIT Kanpur (2013-2016)
- INSA Medal for Young Scientist (2006)

Research:

Dr. Joshi's group is interested in understanding physical behavior and dynamics of structured fluids. His group combines expertise from Chemical Engineering, Physics, Chemistry and Materials Science to understand molecular phenomena that is responsible for the flow behavior. Major thrust area of his group is to understand ageing and effect of deformation on the variety of soft glassy materials such as concentrated suspensions, glassy polymers and polymer nanocomposites. Common theme in all these systems is their jammed state wherein primary entity (particle or molecular segment) is physically arrested due to overall crowding of constituents. In such state, system explores only a small part of the phase space thereby leading to a glassy behavior.

Recently Dr. Joshi's group showed that how rheological characterization can give profound insight into the ageing of colloidal glasses compared to that of colloidal gels. Dr. Joshi's group also investigated effect of deformation on the ageing suspensions and how influence of the same on relaxation dynamics can be used to predict long time rheological behavior of these materials. Dr. Joshi's group is also involved in understanding rheological behavior of discotic nematic suspensions, particularly their intriguing flow behaviors that are industrially very important. Dr. Joshi's group actively consults with industry, including UPL Ltd. and Unilever Inc., regarding improving the flow behavior and rheological stability of their products.

Selected Publications:

1. Y. M. Joshi, Thixotropy, non-monotonic stress relaxation, and the second law of thermodynamics, Journal of Rheology, 66,111 (2022).

2. S. Shanbhag, Y. M. Joshi, Kramers-Kronig Relations for Nonlinear Rheology: 1. General Expression and Implications, Journal of Rheology, 66, 973 (2022).

3. N. Joshi, K. Suman, Y. M. Joshi, Rheological Behavior of Aqueous Poly (vinyl alcohol) Solution During a Freeze-Thaw gelation Process, Macromolecules, 53, 3452 (2020).

4. K. Suman, Y. M. Joshi, Microstructure and Soft Glassy Dynamics of Aqueous Laponite Dispersion, Langmuir, 34, 13079 (2018).

Santosh K. Gupta

Senior Scientist Fellow, NASI

PhD, University of Pennsylvania
Contact: | Email: skgupta@iitk.ac.in

Awards and Honours:

- L & T Chair Professor of Chemical Engineering, IIT Bombay (2009-2010)
- Fellow, Indian National Academy of Engineering (2009)
- Fellow, National Academy of Sciences, India (2005)
- Herdillia Award of the Indian Institute of Chemical Engineers for Excellence in Basic Research (1987)
- Fellow, Indian Academy of Sciences (1987)

Research:

Dr. Santosh K. Gupta is currently a Senior Scientist Fellow, NASI Prayagraj, in the Department of Chemical Engineering, IIT Kanpur, Kanpur, India. He has spent almost his entire academic life at the Indian Institute of Technology, Kanpur, except for short sojourns. He graduated at the head of the entire engineering class in 1968, earning a Bachelor's degree (B. Tech.) in Chemical Engineering from IIT Kanpur. For this achievement he was awarded the President of India's gold medal for the best graduating student. He obtained his master's degree in 1970 and his doctorate in 1972, working with Professor William C. Forsman at the University of Pennsylvania, Philadelphia, U.S.A. After a one-year postdoctoral work with Professor Forsman, he returned to IITK in fall 1973 as an assistant professor in the Chemical Engineering Department. After superannuating from IIT Kanpur (as a professor) in 2012 he joined the University of Petroleum and Engineering Studies (UPES), Dehradun, and contributed to the recruitment of excellent faculty there, organized international conferences and helped get NAAC accreditation for the Department. He is now back at IIT Kanpur.

Professor Gupta has made outstanding theoretical and experimental contributions to the fundamental understanding in the general area of polymerization reaction engineering, and optimization using evolutionary techniques. The research in these areas has led to over 200 research papers in international, high-impact refereed journals. He has a high h-index. He was included in two lists of the most highly cited chemical scientists, with 845 citations received for 117 papers (till 1998). He has been an inspiration and a role model to generations of undergraduate and graduate students. In addition to his research activities, Professor Gupta has taught and developed a wide variety of undergraduate and graduate courses. His student reaction surveys have been extremely laudatory, and year after year, he is being claimed by the students in his class to be one of the best teachers/motivators in IIT Kanpur, IIT Bombay, Mumbai (where he was an L&T Chair Professor for six months) as well as at UPES, Dehradun. His teaching and concern for students have led to the publication of seven well-recognized and quality textbooks for students, one research monograph (Plenum, NY), and two Conference Proceedings. The latest book on Optimization was released in 2021. He has motivated even undergraduate students to do outstanding fundamental research, resulting in publications in reputed international journals. Currently, he with some of his Ph.D. students at UPES Dehradun, is writing a textbook on Process Control for Chemical Engineers.

Selected Publications:

1. R. Mahajan, S. K. Gupta, Modeling of Diffusional Limitations in Styrene Acrylonitrile (SAN) Random Bulk Copolymerization, Polymer Engineering & Science, 55,2098 (2015).

2. R. Mahajan, S. K. Gupta, Optimization of Styrene Acrylonitrile (SAN) Random Bulk Copolymerization Reactors, Polymer Engineering & Science, 55, 2377 (2015).

Arijit Bose

Visiting Distinguished Professor

PhD, University of Rochester
Contact: | Email: bosea@uri.edu
Web:https://web.uri.edu/~

Awards and Honours:

- URITC Researcher of the Year (2012)
- URI Outstanding Researcher Award (2011)
- College of Engineering, Outstanding Researcher Award (2011)
- URI Outstanding Intellectual Property Award (2008, 2004)
- Vincent and Estelle Murphy Award for Faculty Excellence, College of Engineering, University of Rhode Island (2000, 1991)
- Horizons Lecturer, Kimberly-Clark Corporation (1993)
- Summer Faculty Fellow, University of Rhode Island (1986-1990)
- Lilly Teaching Fellow, University of Rhode Island (1985-1986)
- Elon Huntington Hooker Fellow, University of Rochester (1978-1979)
- Graduate Fellow, Department of Chemical Engineering, University of Rochester (1976-1978, 1979-1980)
- National Science Talent Scholar, India (1971)

Research: Our group currently working in three broad areas

(a) Energy storage

We are developing all-solid lithium ion batteries for active implantable medical devices, and for unmanned underwater vehicles, that are much safer than current batteries that contain organic liquid electrolytes. Our strategy is to use a combination of polymer-based electrolytes and active materials to deliver high cycle stability and the power and energy required for these diverse applications. We have developed novel processing strategies for making batteries with silicon-based anodes, and examined the composition and morphology of the growing solid electrolyte interphase layer from graphite and silicon anodes.

(b)Analyte detection in sea and fresh water

We are developing hybrid carbon-gold nanoparticles that can be used for detecting a broad spectrum of analytes using Surface Enhanced Raman Scattering. Our immediate focus is the detection of nitrate and phosphate ions in 'natural' water. This is important because excess nitrates and phosphates in water (typically from fertilizer runoff after storms) cause algae blooms that result in local hypoxia with deleterious consequences on marine and freshwater organisms.

(c)Influence of microplastics on marine and freshwater bacteria

About 150 million tons of plastic are in the world's oceans currently, and 8 million additional tons are dumped into the ocean each year. By 2050, the weight of plastics in the ocean will exceed the weight of all marine organisms. These are highly concerning statistics, since plastics, (mostly polyethylene) in the ocean do not degrade easily, and can impact marine life for over a hundred years. Through ocean action, light and wind exposure these plastics eventually break up into millimeter- and lower-sized objects, or microplastics. Microbeads were also prevalent in personal care products such as exfoliating shower gel, toothpaste, and makeup, which eventually ended up in the ocean. A range of sea creatures, such as oysters and fish, are known to consume these microplastics. with inevitable negative consequences up the food chain.

Selected Publications:

1. Tania T. S. de Oliveira, A. Abbasi, I. Andreu, A. Bose, Plasmon-Tuned Particles for the Amplification of Surface-Enhanced Raman Scattering from Analytes, Langmuir 38 (46) (2022).

2. O. Owoseni, Y. Su, S. Raghavan, A. Bose, V. T John, Hydrophobically modified chitosan biopolymer connects halloysite nanotubes at the oil-water interface as complementary pair for stabilizing oil droplets, Journal of Colloid and Interface Science, 620 (2022).

Former Faculty

Prof. Avadh B. Agarwal
(1964-2000)

Prof. P. K. Bhattacharya
(1977-2016)

Prof. R. P. Chhabra
(1984-2018)

Prof. Jagdish K. Gehlawat
(1975-1997)

Prof. Jai P. Gupta
(1972-2010)

Prof. Santosh K. Gupta
(1973-2012)

Prof. Ashok Khanna
(1982-2013)

Prof. Anil Kumar
(1972-2012)

Prof. Deepak Kunzru
(1975-2016)

Prof. Davuluri P. Rao
(1976-2005)

Late Prof. Musti S. Rao
(1971-2003)

Late. Prof. Y.V.C. Rao
(1964- 2004)

Prof. Deoki N. Saraf
(1967-2003)

Prof. Rakesh P. Singh
(1966-2004)

Prof. K. S. Gandhi
(1963-1986)

Research and Administrative Staff


Dr. Debjani Banerjee
Senior REO


Mr. Abhishek Mishra
REO


Shri Ram Ashish Mishra
Senior Technical Superintendent


Shri Rajiv K Yadav
Senior Technical Superintendent


Shri Deepak Ubale
Senior Technical Superintendent


Shri R.K. Vishwakarma
Technical Superintendent


Shri Naveen Kumar Gupta
Technical Superintendent


Shri Rajesh Kumar Tiwari
Superintendent


Shri Rajesh Kumar Singh
Technical Superintendent


Shri Vijay Kumar
Senior Technician


Shri S. K Kanaujia
Senior Technician


Shri Saroj.K. Rawat
Senior Technician


Shri Abhishek Gaur
Senior Technician


Shri Krishnendra Tripathi
Senior Technician


Shri Anand Kumar Singh
Senior Assistant


Mrs. Pallavi Gautam
Senior Assistant


Shri Dhirendra Kumar
Senior Technician


Shree Shubham Saxena
Junior Technician


Sandeep Kumar
Junior Technician


Ramu
Junior Technician

Department Research Facilities

Post Graduate Research Laboratory (PGRL) is a user facility in the Department of Chemical Engineering at IIT Kanpur that supports a broad range of science and technology projects by merging state-of-the-art resources with expert support staff. PGRL provides research space, sophisticated instruments and services thereby imparting an able platform for academic and industrial researchers to develop applications and expertise dedicated to addressing variety of scientific and engineering challenges. In-house equipments at PGRL include :

- High Resolution Field Emission Scanning Electron Microscope (FESEM)
- Inductively Coupled Plasma-Mass Spectrometer (ICP-MS)
- Thermal Analyzers: Thermogravimetry (TGA) & Differential Scanning Calorimetry (DSC)
- Automated Gas Adsorption Set up for Physisorption, Chemisorption & Temperature Programmed Oxidation, Reduction & Desorption processes.
- Electrochemistry set up with potentiostat /Galvanostat.
- Powder & Thin film X-ray Diffractometer
- Micro Particle Image Velocimetry (MPIV)
- Universal Testing Machine (UTM).
- Electrospinning Unit with 3D Bioprinter as Accessory.
- Polarization Microscope with Fluorescence spectroscopy & Peltier Stage attachment.

Jeet Bindra Unit Operations and Innovation Laboratory

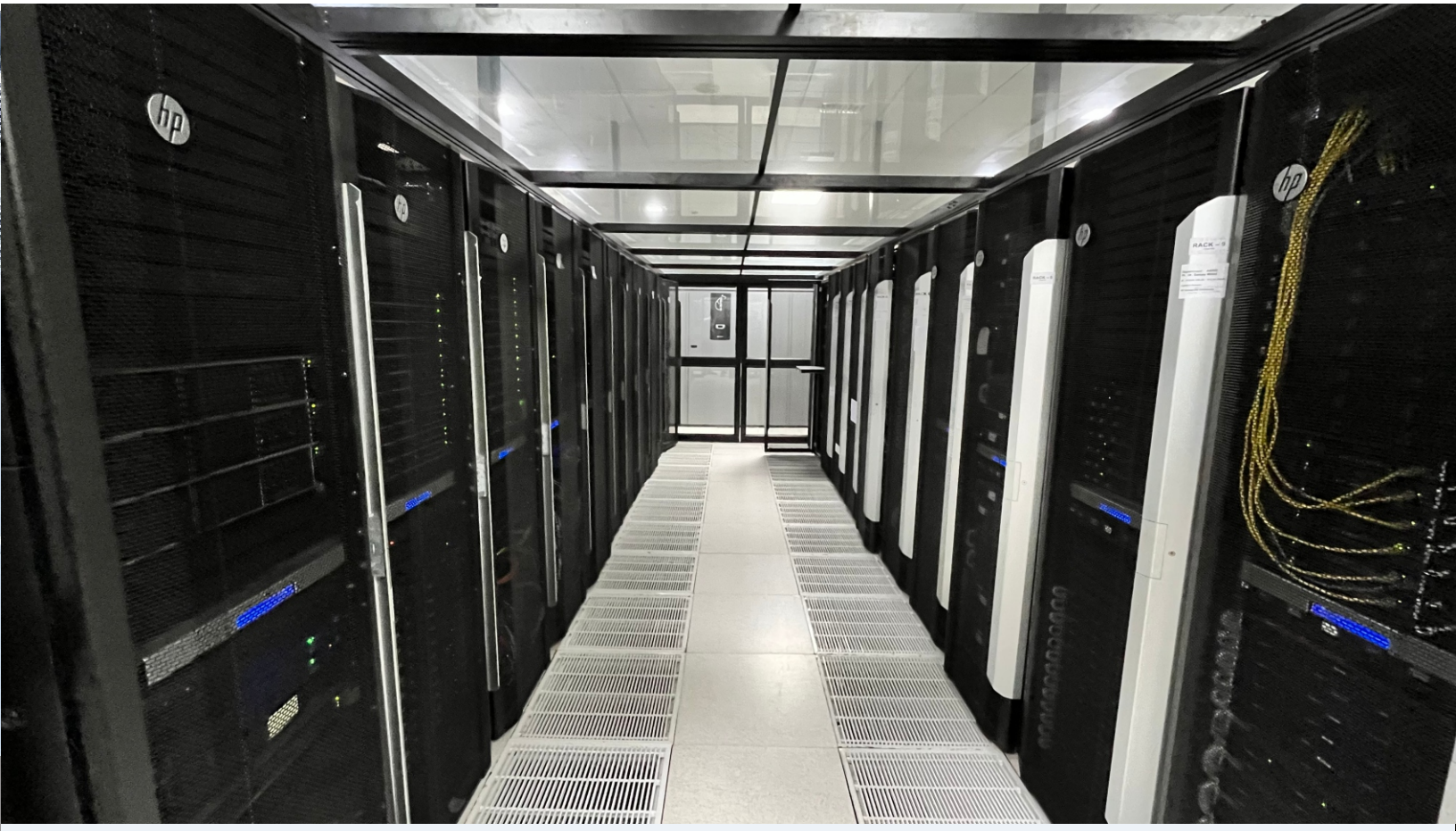
Shri Jagjeet Singh Bindra, our illustrious alumnus and Institute fellow, made substantial contributions, both financially and intellectually, towards the creation of the "Jeet Bindra Unit Operations and Innovation Lab". Due to his diligence and vision, the chemical engineering department can boast of a state-of-the-art laboratory.

Inaugural function of Jeet Bindra Unit Operations and Innovation Laboratory : Professor Abhay Karandikar, Director, IIT Kanpur along with Shri Jagjeet Singh Bindra, our illustrious alumnus and institute fellow and Professor Jayant K. Singh, HoD ChE.

- Enriches UG students with experience that prepares them to hit the ground running. Students work in teams to plan and conduct experiments, collect and analyze data, and write technical reports.
- Goal is to transform students from stand-alone homework-solvers, and test-takers into communicators, team-members, and open-ended problem solvers.

- UOP is based on exciting capstone courses on core areas of thermodynamics, fluids, separation, heat and mass transfer, reaction engineering and process control. New equipments, connected experiments augmented with simulation and modelling has been able to create more cohesive experience for UG-students.
- Chemical Engineering seniors are encouraged to build teamwork skills in a state-of-the-art environment. Features bench scale unit operations experiments focused on fluid flow, heat transfer, membrane separation, kinetics, liquid extraction, flow measurement and other chemical processes.
- Complements classroom lectures with practical training for 3rd and 4th year UG students. Practical skills such as these prove to be indispensable on a graduate's first job in industry.
- Opportunity to learn in a real-world chemical-processing work environment providing a practical, hands-on experience.

High Performance Computing (HPC) Facility



HPC systems at Computer Center, IIT Kanpur, are greatly facilitating high-end computation research in the country covering many areas of science and engineering. IIT Kanpur already has 2 HPC clusters, known as HPC 2010 and HPC 2013. The 372-node HPC 2010 cluster is based on Intel Xeon Quadcore processors with a total of 2944 cores and high-speed Infiniband network, and it has a peak performance of 34.5 Teraflops. The 899-node HPC 2013 cluster is also based on Intel Xeon processors and has 17980 cores in total, and peak performance of 360 Teraflops. On the infrastructural side, a modern data centre with state-of-the-art precision air conditioning and fire safety features is part of the Computer Centre.

3D Bio Printing Facility

Student Life

IIT Kanpur is a fully residential campus with all students being provided on-campus accommodation spread across 12 Halls of Residence. Each Hall has well-furnished kitchen and dining facilities, canteens, a computer facility, a reading room, LAN connectivity in the rooms along with sprawling lawns for prolonged bulla (chit chat) sessions. These provide for a very cosy on campus stay where life-long friendships are formed. Campus life teems with the exuberance and vitality of youth. Each Hall has its own sports infrastructure for a game of phatta cricket, volleyball, basketball, table tennis, outdoor badminton to name few. For the more serious ones, we have state-of-the-art indoor and outdoor sports facilities and a gymnasium. Students also express their talents through membership and participation in activities of various clubs such as aeromodeling, music, ham-radio, photography, adventure sports amongst many others.There exists a very liberal campus environment for students to discover and explore their inner calling. The guiding philosophy is to treat them as adults and give them the flexibility to make their own choices from the very beginning, which naturally matures them into responsible individuals balancing professional and personal pursuits.

Career Avenues:

ChE@IITK attracts some of the best student talent in the country so that our students are naturally highly sought after by industry (Private / Government) and academia. The campus has a Placement office for on-campus recruitment. The placement season usually begins on December 1

every year across all IITs. Most students get placed in the month of December. Several students also go abroad on scholarship for higher studies. Our PhD students are highly sought after for post-doctoral research, industrial R&D and by academic institutes.

Graduating Batch Award Winners:

Amrita Goswami

Outstanding PhD Thesis Award

PhD, Chemical Engineering
2016-2021

Lakshay Tyagi

Best Academic Performance amongst graduating students of 4 year/5 year UG Programme

Bachelor's degree, Major in Electrical Engineering and Chemical Engineering, Minor in Computer Science
2017-2022

Deeksha Yadav

IIT Kanpur Excellence Awards in Community Services,

Best UG Project Work amongst graduating students of 4 year/5 year UG Programme

BTech-MTech Dual, Chemical Engineering
2017-2022

Aakash Soni

IIT Kanpur Excellence Award in Art and Cultural Activities

BTech, Chemical Engineering
2018-2022

Sunamya Gupta

Shrimati Tarad Dube and Shri Raj Deva Dube Memorial Gold Medal for the best academic performance in 4 year/5 year programmes of the Chemical Engineering Department

BTech, Double major : Chemical Engineering and Electrical Engineering
2017-2022

Kopparthi Venkata Srita

Best All Rounder Girl Student of two year masters programme Gold Medal

Mtech, Chemical Engineering
2020-2022

Vedaant Sikka

Awarded the IITK Excellence for Leadership in Student Affairs

BTech, Chemical Engineering
2018-2022

Amisha Shahdeo

Shri Ghisa Lal Kamdar Memorial Medal for the best outgoing 4 year undergraduate student of the Chemical Engineering Department

BTech, Chemical Engineering
2018-2022

Chemineers Society @ IITK:

Chemineers Society IIT Kanpur helps students to identify campus resources and foster harmonious relationship among students, faculties, and administration of the Chemical Engineering Department. The society organizes a wide range of activities for the benefit of the Chemical department community at IIT Kanpur. These activities range from fun filled happy hours to large symposiums.

Prospective Faculty

The Department of Chemical Engineering at IIT Kanpur is ranked among the nation's top schools in Chemical Engineering, and is endowed with a vibrant graduate program, a distinguished faculty that has earned national and international honors, and a well-regarded undergraduate program. Aside from excellence in fundamental research, the department has made significant contributions to the chemical industry through its expertise in chemical process engineering, simulation, optimization and control, polymers, interfacial phenomena and separations, including membrane separations. There has been a long tradition in the department to write quality text-books and research monographs, and over 32 books have been published by both Indian and International publishers. Our alumni, many of who have gone on to be the CEOs, business leaders, department chairs and distinguished scientists (even social workers and artists!), both in India and abroad, are a very visible lot and continue to inspire the new generation of students here. The department has been continually adapting and responding to the rapidly changing economic, social and technological scenarios at the national and international levels in the last several years.

Experimental research in the department is supported by state-of-the-art facilities which include scanning tunneling and atomic force microscopes, ellipsometer, contact angle goniometer, Langmuir-Blodgett deposition, atomic absorption spectrophotometer, FTIR, GPC, rheometers, HPLC, several membrane cells, high performance computing clusters with chemical process simulation software such as ASPEN and HI-SYS. State of art computational research facilities are also available for gene expression profiling/gene network analysis, and for molecular simulations, etc. The department hosts a nano-technology center. A new facility for the measurement of NO x concentrations in air over a range of 10 – 10,000 ppm by a dedicated chemi-luminescence analyzer has been created. Several projects funded by industry and spanning a wide spectrum of areas are currently underway. These include those from Unilever India, Bangalore, Chevron-Texaco Inc, USA , and Gas Authority of India (GAIL) and quite a few medium-sized private industries, etc.

The Institute has a self-contained campus located in a beautiful wooded land. The campus offers a peaceful and modern lifestyle to the faculty, staff and their families and is a great place for children to grow up with excellent schools and a stimulating environment. The facilities and research atmosphere in our department supports its faculty in building successful teaching and research careers. Moreover, the Institute has excellent infrastructure available in individual departments and centres; and has several centrally located facilities for researchers.

As a faculty member you will join the community of highly motivated scholars both within your department and beyond it, with several opportunities in cross-disciplinary collaboration. On-campus housing is available for faculty. There are a several types of housing ranging from bungalows and apartments of various sizes; which are allocated by the Estate office based on eligibility. Internet connectivity is available in the residences. Health care facility is provided by the Institute through the hospital on campus. Resident physicians are available 24/7 and visiting specialists are available at different times in the day. There are several facilities within the campus for faculty and their families such as Shopping Centres, Banks, Post Office, Schools, Day Care Centre, etc. The Institute has a good number of sport facilities - football, tennis, basketball, hockey, skating, badminton court, swimming and a stadium matching international standards. There are exclusive tennis and basketball courts for the staff of the Institute. The Student Activities Centre houses the volleyball and the badminton courts as well as the indoor basketball court. The Gymnasium has state-of-the-art facilities.

Acknowledgements: Dr. Jayant K Singh,
Dr. Himanshu Sharma, Dr. Rahul Mangal,
Dr. Harshwardhan H. Katkar, Dr. Dipin S. Pillai,
Dr. Raghavendra Ragipani, Dr. Debjani Banerjee
Photo Credits: Mr. Krishnendra Tripathi
Design: Mr. Abhishek Mishra

IIT KANPUR

Department of Chemical Engineering

IIT Kanpur, Kanpur 208016 (U.P.), India.