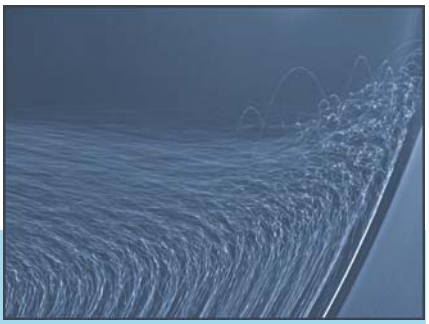
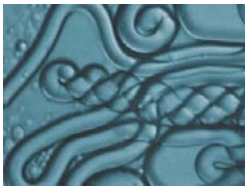


Department of Chemical Engineering

Indian Institute of Technology, Bombay



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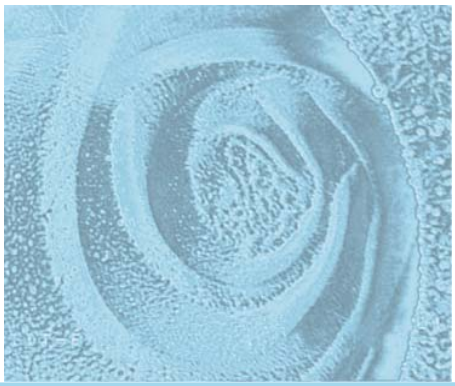


mission statement

Education

A compact and effective undergraduate program that gives an comprehensive exposure to fundamentals and to industrial application of concepts. A dynamic postgraduate program with opportunities and strong emphasis on basic and applied research in a wide range of areas.

Research

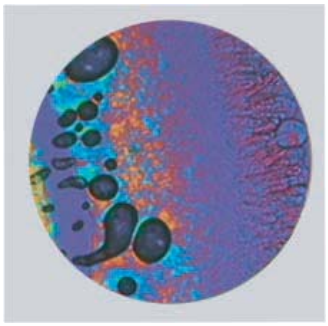
A dynamic research program generating new concepts and ideas that have a significant and lasting impact on industrial practice and contribute to the fundamentals of Chemical Engineering.

Industry Interaction

To emerge as a Knowledge Sharing Center of Excellence in selected areas of expertise which becomes the natural choice of Process Industry for assistance in problem solving.

Alumni Interaction

To enhance the goodwill and to build a strong support group among alumni for Departmental Programs.



Department of Chemical Engineering
Indian Institute of Technology - Bombay
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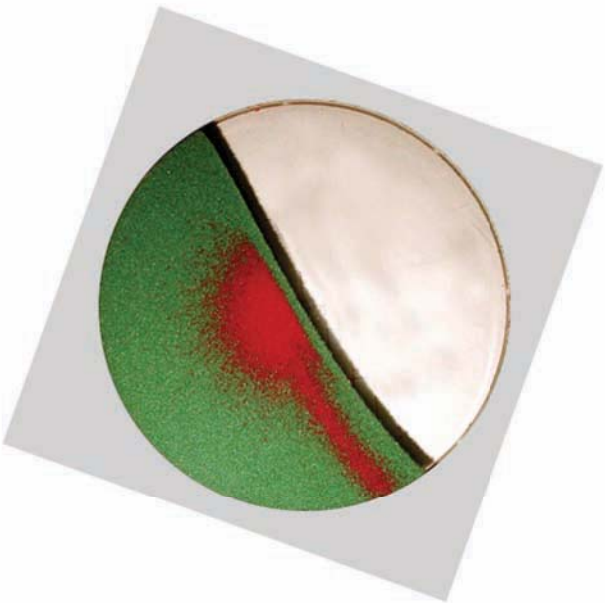


message from HOD

Chemical Engineering, in essence, concerns the economic design and operation of chemical plants. Today, chemical plants encompass a considerable range. For example, computer chip manufacturing units, engineered micro-organisms for pharmaceuticals, engineered ecosystems for environment upgradation and drug delivery systems are some of the "new" chemical plants which coexist with the "traditional" chemical plants for manufacture of basic chemicals, petroleum, polymers, pharmaceuticals, cement, fertilizer and processed foods. Chemical Engineering fundamentals draw from physics, chemistry, mathematics and increasingly biology, which is combined with engineering art to understand and control molecular and macroscopic processes in these diverse systems. The discipline is expanding and the new science and engineering are helping develop technologies that are more efficient, safer and environmmentally friendly. Chemical Engineers have made important contributions to society over the years in terms of products and processes. The breadth and versatility of their training will continue to open many new opportunities for chemical engineers in the future.

The Chemical Engineering Department at I.I.T. Bombay is committed to excellence in Chemical Engineering education in the context of the evolving discipline. The Department has a strong core curriculum complemented by electives in the important emerging areas, at both undergraduate and postgraduate levels. Research is an important focus of activity and the Department has an excellent faculty who lead high quality research programmes in a wide spectrum of areas. The Department is provided with very good experimental facilities for research and a strong technical staff. The Department has strong links with industry with interactions spanning consultancy, sponsored research and continuing education. The alumni are important stakeholders and have provided generous support in different ways.

Our mission is to create and sustain an environment for learning, enquiry and generation of new ideas to aid the education of chemical engineers who will lead the profession, in the development of new technologies and in the service to the industry.

Prof. Anurag Mehra
(Head of Department)

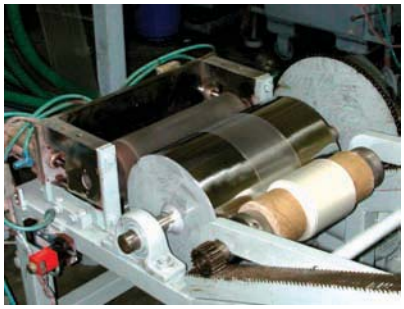
April 1, 2008

about the department

The Department of Chemical Engineering at I.I.T. Bombay was established in 1958, with assistance from the Soviet Union under a UNESCO aid scheme. Initially it was organized on the basis of specializations with distinct laboratories and academic programs. The main areas of research involved Unit Operations (Heat Transfer, Mass Transfer and Fluid Mechanics), Automation in Chemical Industries, Processes (Inorganic and Organic) and Technologies (Fuel, Silicate, Cellulose and Electrochemical). Over the years, the Department has diversified into several contemporary areas of research, with an emphasis on chemical engineering fundamentals. The overall academic program today reflects this status. However, specialization in particular sub-disciplines is possible by through streamed electives and research projects.

Today the Department is recognized as a leading one in India, primarily because of its strong academic program, large faculty strength and the breadth of their research areas. Several faculty members of the Department also participate in teaching and research activities of various interdisciplinary programs of the Institute. The Department today boasts of a wide range of sophisticated experimental and computational facilities, built up through infrastructure-support grants and research projects from various governmental agencies (MHRD, DST, CSIR, DBT, etc.) as well as the industry. Currently, the department has about 350 undergraduate students, and over 200 postgraduate students (including research scholars).

The Department has established, and continues to nurture an effective rapport with the industry. It provides services related to varied technologies by way of consultancy projects and continuing education courses. The intensity of the R&D engagement and industry-interaction of the department has been growing steadily over the years.



Isothermal Microcalorimeter
Organic Process Laboratory

Academic Programs:

The heart of the Chemical Engineering program at IIT Bombay is excellence in undergraduate and post-graduate education. Our programs aim to impart students the ability to conduct innovative research and to inculcate the sprit of scholarship. Students are encouraged to play an active role in formulating the research to be undertaken, implementing the work, and carrying it to completion. The post-graduate research projects aim to synthesize fundamental study of technologies with an emphasis on their practical significance. The academic programs of the department include B.Tech. (4 year duration), Dual Degree (5-year duration), M.Tech. (2 year duration) and the Ph.D. program.

B.Tech. Program

Core Courses

CL 152 Introduction to Chemical Engineering
CL 203 Introduction to Transport Phenomena
CL 240 Materials Technology
CL 251 Thermodynamics I
CL 252 Thermodynamics II
CL 256 Fluid and Fluid-Solid Operations
CL 248 Heat Transfer Operations
CL 322 Kinetics
CL 351 Mass Transfer I
CL 352 Mass Transfer II
CL 353 Mathematical and Computational Techniques for Chemical Engineers
CL 354 Process Equipment Design and Economics
CL 358 Instrumentation and Process Control
CL 421 Reaction Engineering
CL 441 Chemical Processes I
CL 442 Chemical Processes II
CL 451 Chemical Process Design

Laboratory Courses

CL 232 Chemical Engineering Laboratory I
CL 333 Chemical Engineering Laboratory II
CL 335 Chemical Engineering Laboratory III
CL 332 Chemical Engineering Laboratory IV
CL 334 Chemical Engineering Laboratory V
CL 431 Chemical Engineering Laboratory VI

Departmental Electives

CL 356 Process Plant Utilities
CL 360 Introduction to Cryogenic Engineering
CL 402 Project Engineering
CL 420 Introduction to Biochemical Engineering
CL 424 Heat Exchanger Network Design
CL 444 Safety in Chemical Industry
CL 461 Introduction to Colloidal and Interfacial Science & Engineering
CL 463 Introduction to Food Engineering
CL 465 Stochastic Processes
CL 484 Electrolytic Cells

Dual Degree Program (B.Tech. + M.Tech.)

Core Courses (In addition to B.Tech. courses)

CL 603 Optimization
CL 687 Artificial Intelligence in Process Engineering
CL 684 Advanced Process Synthesis
CL 686 Advanced Process Control
CL 676 Modelling and Simulation

Laboratory courses

CL 216 Computational Laboratory I
CL 316 Computational Laboratory II
CL 453 Computer Aided Design Laboratory

M.Tech Program/Ph.D. Program

Core Courses

CL 601 Advanced Transport Phenomena
CL 602 Mathematical & Statistical Methods
CL 605 Advanced Reaction Engineering
CL 607 Advanced Thermodynamics
CL 610 Experimental Methods
HSS 699 Communication Skills
CL 701 Computational Methods in Chemical Engineering

Departmental Electives

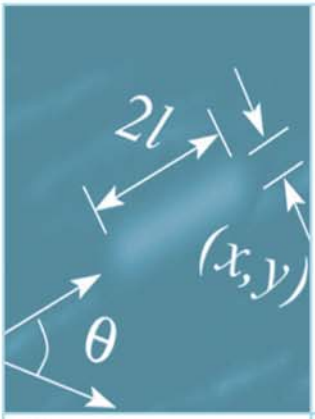
CL 609 Pollution Control Systems
CL 611 Electrochemical Reaction Engineering
CL 624 Polymer Processing
CL 644 Modeling and Analysis of Bioprocesses
CL 647 Advanced Process Optimization
CL 649 Reaction Engineering in Dispersed Phase systems
CL 650 Process Monitoring and Fault Diagnosis
CL 676 Modelling and Simulation
CL 688 Artificial Intelligence in Process Engineering
CL 705 Bioseparations

research areas

A wide range of topical areas in chemical engineering and its allied fields is actively being researched by the departmental faculty. The research problems range from fundamental studies relating to the microscopic domain such as particle dynamics of granular flows and microstructure of micelles and liposomes, to applied research like pilot studies for supercritical extraction of natural products and application of vermiculture to waste processing. The research is often multidisciplinary and involves active collaboration between faculty within the department and institute, and with researchers from other universities and research establishments, as well as industrial R&D laboratories. A broad classification of research areas is given in the following page, along with faculty working in these areas. Specific details for each faculty are given in the following pages.

Fermentor
Protein Engg. Laboratory

Reactive Distillation System
Reaction Engineering Laboratory



	Biosystems Engineering	Systems Engineering & Control	Interface Science & Engineering	Separation Science	Polymers & Materials	Food Engineering	Catalysis & Reactor Engineering	Environmental Engg & Safety	Fluid and Particle Mechanics
Adhikari Jhumpa					•				
Aghalayam Preeti							•	•	
Bandyopadhyaya R.			•		•				
Bellare J.R.	•		•	•					
Bhartiya Sharad	•	•							
Bhushan Mani	•	•						•	
Gudi R.D.	•	•							
Jadhav S. R.	•		•						•
Juvekar V.A.			•	•	•		•		
Khakhar D.V.					•				•
Khilar K.C.			•						•
Mahajani S.				•		•	•		
Malik R.K.		•		•					
Mehra A.			•		•	•	•		
Mehra S.	•								
Misra A.					•				
Moharir A.S.		•		•			•		
Moudgalya Kannan M		•							
Mukhopadhyay M.				•		•			
Nanavati H.					•				
Noronha Santosh	•	•					•	•	
Patwardhan Sachin		•							
Rao V.Govardhana				•				•	•
Roy S.			•	•	•			•	
Shankar H.S.	•						•	•	
Suresh A.K.	•				•		•		
Sunthar P.			•		•				•
Thaokar R.			•		•				•
Tirumkudulu Mahesh			•		•				•
Venkataraman Chandra			•					•	•
Venkatesh K.V.	•	•				•			
Vinjamur Madhu			•		•	•			•
Viswanathan G. A.	•						•		
Wangikar P.	•	•							•

faculty

Jhumpa Adhikari (Ph.D., U. at Buffalo, 2004)

Preeti Aghalayam (Ph.D., U. Massachusetts, 2000)

Rajdip Bandyopadhyaya (Ph.D., IISc Bangalore, 2000)

Jayesh Bellare (Ph.D., U. Minnesota, 1988)

Sharad Bhartiya (Ph.D., Oklahoma State U., 2000)

R. D. Gudi (Ph.D., U. Alberta, 1995)

S.R. Jadhav (Ph.D., Johns Hopkins U., 2004)

V. A. Juvekar (Ph.D., U. Bombay, 1976)

D. V. Khakhar (Ph.D., U. Massachusetts, 1986)

K. C. Khilar (Ph.D., U. Michigan, 1981)

Mani Bhushan (Ph.D., I.I.T. Bombay, 2001)

Sanjay Mahajani (Ph.D., U. Bombay, 1996)

R. K. Malik (Ph.D., U. Wisconsin, 1979)

A. Mehra (Ph.D., U. Bombay, 1987) **(Head of the department)**

S. Mehra (Ph.D., U. of Minnesota, 2005)

A. Misra (Ph.D., U. Massachusetts, 1974)

A. S. Moharir (Ph.D., I.I.T. Kanpur, 1981)

Kannan M. Moudgalya (Ph.D., Rice, 1985)

M. Mukhopadhyay (Ph.D., Ohio State U., 1969)

Hemant Nanavati (Ph.D., Georgia Tech, 1998)

S. Noronha (Ph.D., U. Maryland, 1996)

S. C. Patwardhan (Ph.D., I.I.T. Bombay, 1994)

V. Govardhana Rao (Ph.D., I.I.T. Madras, 1979)

Sandip Roy (M.S., SUNY, Buffalo, 1982)

H. S. Shankar (Ph.D., Monash U., 1976)

A. K. Suresh (Ph.D., Monash U., 1986)

P.Sunthar (Ph.D., IISc Bangalore., 2002)

Rochish Thaokar (Ph.D., IISc Bangalore., 2003)

Mahesh S. Tirumkudulu (Ph.D., City University of New York, 2001)

Chandra Venkataraman (Ph.D., U. of California, Los Angeles,1992)

K. V. Venkatesh (Ph.D., Purdue U., 1993)

Madhu Vinjamur (Ph.D., Drexel University, 2001)

Ganesh A Viswanathan (Ph.D., University of Houston, Houston, 2004)

P. Wangikar (Ph.D., U. Iowa, 1995)

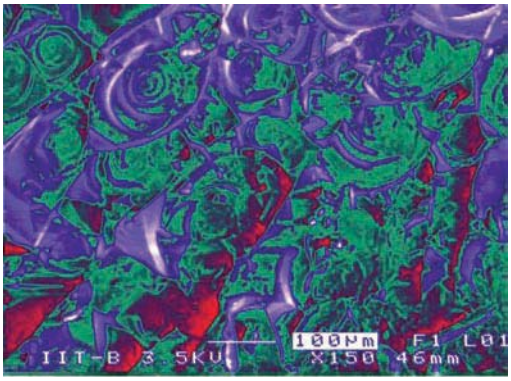
Adjunct Faculty

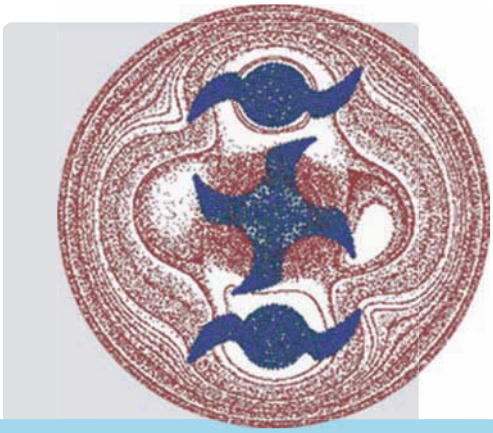
S. G. Kane (Ph.D., MIT, 1971)

S. Ganesan (Ph.D., I.I.T. Bombay, 1980)

Janaky Narayanan (Ph.D., U. of Bombay, 1995)

V.M. Naik





Jhumpa Adhikari

B.E. R.E.C., Durgapur, 1997
Ph.D., University at Buffalo, The State University of New York, 2004
adhikari@che.iitb.ac.in

Molecular Thermodynamics, Statistical Mechanics, Molecular Simulation

Molecular Simulations techniques are used in the development of new methods for determination of free energies and phase equilibria. Simulation of solids provide unique challenges because of the high densities involved which preclude use of many of the well established methods used in the fluid phases. This provides an opportunity for the development of new methods to successfully measure the free energy of the solids and to improve the efficiency of the techniques used.

The application and continued development of java package called "etomica" (DAK group, University at Buffalo) for molecular simulations.

Design of compound semiconductor alloys using molecular simulation:

Molecular simulation techniques are applied to determine the miscibility diagrams for solid solutions, such as ternary and quaternary compound semiconductor alloys, and also to study the structure-property relations while providing explanation of the underlying molecular mechanism.

Molecular Simulation determination of phase equilibria and interface properties of metals:

Prediction of properties, that are consistent with the inter-particular forces, for metals at extreme conditions where metals often show morphologies which are not as observed at room conditions by using molecular simulations;

Selected Publications:

- Adhikari, Jhumpa and A. Kumar, Study of structural and thermodynamic properties of GaAs and InAs using Monte Carlo simulations. Molecular Simulation (2007), 33(8), 623-628
- Singh, J. K., Adhikari, J and S. K.Kwak, Vapor-liquid phase coexistence curves for Morse fluids. Fluid Phase Equilibria (2006), 248(1), 1-6
- Adhikari, J and D.A.Kofke, Molecular simulation study of miscibility of ternary and quaternary semiconductor alloys. Journal of Applied Physics (2004), 95(11), 6129-6136
- Lu, Nandou; Adhikari, J and D.A.Kofke, Variational Formula for the Free Energy Based on Incomplete Sampling in a Molecular Simulation. Physical Review E: Statistical, Nonlinear, and Soft Matter Physics (2003), 68(2-2)

Preeti Aghalayam

B.Tech., I.I.T., Madras, 1995.
M.S., University of Rochester, Rochester, NY, 1996.
Ph.D., University of Massachusetts, Amherst, U.S.A., 2000.
Post Doc, Massachusetts Institute of Technology, Cambridge, MA
preeti@che.iitb.ac.in

Underground Coal Gasification, Development of Detailed Surface Reaction Mechanisms, Automotive NOx Control

Underground Coal Gasification :

The in-situ gasification of deep coal deposits has great potential for enhancing energy supply for the country. A systematic chemical engineering approach is being taken in order to understand the various complex phenomena in UCG. The focus is on the occurrence of multiple reactions, determination of appropriate kinetic equations, study of flow patterns, and modelling of coal cavity formation/growth.

Reduction of Automotive NOx:

The catalytic converter is currently widely used for the control of pollutants forming in automobile engines. This multi-purpose device is useful in oxidation of hydrocarbons and carbon monoxide, and also the reduction of Nitrogen Oxides. However, its applicability to diesel, CNG, and lean-burn petrol engines is limited. The focus in our group is on quantification of the relevant catalyst reaction pathways, discrimination between various catalysts from among Platinum Group Metals, and improvements to ensure wider applicability.

Selected Publications:

- D. Mantri, P. Aghalayam, Detailed Surface Reaction Mechanism for Reduction of NO by CO, Catal. Today,119, 98-93 (2007)
- D. Mantri, P. Aghalayam, Micro-kinetic Model for NO reduction on Pt Group Catalysts, Int. J. of Chem. React. Engg., V5, A1 (2007).
- D. Mantri, V. Mehta & P. Aghalayam, Bifurcation Analysis of Pt and Ir catalysts for NO reduction, Canad. J. of Chem. Engg., vol. 85, 333 (2007).
- A. Khadse, M. Qayyumi, S. M. Mahajani & P. Aghalayam, Underground Coal Gasification: A New Clean Coal Utilization Technique for India, Energy, vol. 32, 2061, (2007).
- A. Khadse, M. Qayyumi, S. M. Mahajani & Preeti Aghalayam, Reactor model for Underground coal gasification channel, Int. J. of Chem. React. Engg., V4, A37 (2006).

Rajdip Bandyopadhyaya

B. E., Chem. Engg., Jadavpur University, Calcutta, 1992
M. E., Chem. Engg., Indian Institute of Science (IISc), Bangalore, 1994
Ph. D. IISc, Bangalore, 2000
Post Doc, Ben-Gurion Univ. of the Negev, Beer-Sheva, Israel, 2000-2001
Post Doc, Materials Sc. & Engg., Univ. of Utah, Salt Lake City, USA, 2001-2002
Post Doc., Univ. of California at Los Angeles, Los Angeles, USA, 2002-2003
rajdip@che.iitb.ac.in

Colloids, Nanomaterials, Aerosols, Molecular simulations

Nanoparticles: We perform colloidal synthesis and measurements of CdS, Fe3O4, Ag, ZnO and CdS-ZnS core-shell nanoparticles for understanding mechanism of nanoparticle formation. These are being developed as super-paramagnetic contrast agents, biocides in water purification etc. among other applications. Simultaneously, we have formulated population balance models and Monte Carlo simulation schemes to gain predictive insights into these mechanisms, encompassing both spherical and anisotropic inorganic nanostructures.

Mesoporous materials:
Experiments are carried out in making mesoporous silica materials for understanding structure and related adsorption and diffusion issues in nanometer-sized pores as a function of pore diameter. Work is underway on extending these studies to make chemical sensors. Silica-polymer and polymer-nanotube composites for enhanced mechanical properties, smart and switchable membranes, modelling and measurement of indoor and outdoor aerosols are other current and active research areas.

Selected Publications:

- Ethayaraja, M., Bandyopadhyaya, R., Population balance models and Monte Carlo simulation for nanoparticle formation in water-in-oil micro-emulsions: Implications for CdS synthesis, J. American Chemical Society, 2006, 128(51), 17102-17113.
- Ethayaraja, M., Ravikumar, C., Muthukumaran, D., Dutta, K., Bandyopadhyaya, R., CdS-ZnS core-shell nanoparticle formation: Experiment, mechanism and simulation, J. Physical Chemistry C, 2007, 111(8), 3246-3252.
- Ethayaraja, M., Bandyopadhyaya, R., Mechanism and Modeling of Nanorod Formation from Nanodots, Langmuir, 2007, 23(11), 6418-6423.
- Singh, R. K., Garg, A., Bandyopadhyaya, R., Mishra, B. K., Density Fractionated Hollow Silica Microspheres with High-Yield by Non-Polymeric Sol-Gel/Emulsion Route, Colloids and Surfaces A, 2007, 310(1-3), 39-45.
- Kulkarni, M. M., Bandyopadhyaya, R., Sharma, A., Janus silica film with superhydrophobic and hydrophilic surfaces grown at oil-water interface, J. Materials Chemistry, 2008, 18(9), 1021-1028.

Jayesh Bellare

B.Tech., I.I.T. Bombay, 1982.
Ph.D., U. Minnesota, Minneapolis, U.S.A., 1988.
Post Doc, Materials Science, M.I.T., Cambridge, U.S.A., 1990.
jb@che.iitb.ac.in

Nanotechnology and microengineering;Microstructured materials, devices and processing surfactants, ceramics, polymers, membranes,soft solids & complex liquids; Cryo-electron andoptical microscopy; Image processing;Technical photography; Prototyping, Instrumentation

Liposome and vesicle micr-oreactors: Liposome and vesicle microreactors, their microstructure, deformability under shear, and reactions in them to produce ultrafine particles.

Electron Microscopy of Complex Fluids: Electron Microscopy of Complex Fluids, including development of new microscopy techniques. Morphology of soft solids and complex liquids.

Membrane Technology: Membrane Technology, including composite, supported, asymmetric, hollow-fiber, and ceramic membranes; their preparation, industrial manufacture and characterization.

Artificial organs: Blood oxygenerators, dialysers; new designs and industrial prduction

Ceramic materials: Their pre-cursors, powders and mem- branes; microstructure development; optical properties; bioglasses.

Micro-chemical engineering: Specialized instrumentation, process miniaturization and intensification. Excellent facility set up for cryo-scanning electron microscopy and sample preparation of soft solids and complex liquids; and for Thermal conductivity of fluids: applied to vegetable oils, suspensions and soft solids.

Industry interaction:
Retainer consultant to several companies. Over 15 projects in these areas. Several products / processes are commercialized. Over 12 Patents.

Selected Publications:

Jayesh, B., Srivastava, A. and Menon, A., "Electron microscopy of modified aluminum alkoxide microstructures on freeze drying", J. Coll. Interface Sci., 191,521-524 (1997).

- Jayesh, B., Haridas, M., Menon, A., Goyal, N. and Chandran, S., "Cryogenic-Scanning Electron Microscopy as a technique to Image sol-to-gel transformation in chelated alkoxide systems", Ceramics International, 22,155-159 (1996).
- Jayesh, B., Shah, P.B., and Bandopadhayay, S., "Environmentally degradable starch filled low density polyethylene", Polymer Degradation and Stability, 47, 165-173 (1995).

Society, 54, 149 (1995).
Jayesh, B., Menon, A., Prabhu, C.S., Haridas, M. and Mohan, T.R.R., "Insitu formation and imaging of cellular alumina in a Cryo-SEM environment", Journal of Materials Science Letters, 16, 1506 (1997) Cover Page Article) 522-532 (1997).

Sharad Bhartiya

B.E., REC, Durgapur, 1991.
M.Tech., I.I.T., Madras, 1993.
Ph.D., Oklahoma State University, 2000.
bhartiya@che.iitb.ac.in

Modeling, Control and Estimation of Hybrid Systems, Numerical Optimization, Optimal Control of Large Scale Distributed Parameter Systems, Control of Pulp Digester, Engineering Principles in Biological Systems

Hybrid systems:
Modeling, optimization and control of dynamic hybrid systems; development of efficient MINLP algorithms based on reduced-space methods for predictive control of hybrid systems; mixed integer dynamic optimization; identification of multiple linear models for hybrid systems; optimal state estimation strategies for piecewise affine systems

Distributed Parameter Systems - Pulp Digester:
Management of property profiles in DPS; inferential, multi-rate control of Kappa profile using EKF and MPC; lexicographic optimization strategies to prioritize degrees of freedom in control of DPS; optimal grade transition (hardwood/softwood); first principles models for pulping of wheat straw in a Pandia® digester; corelation models for online Kappa measurement

Systems Biology: Characterization of regulatory architecture of tryptophan system in Escherichia coli; evolutionary differences in regulation of GAL system in yeasts; modeling of cell cycle in fission yeast;

Selected Publications:

- N. Nandola and S. Bhartiya , "A multi-model framework for control of hybrid systems", Journal of Process Control, 18, 131-148 (2008).
- S. Bhartiya, N. Chaudhary , K.V. Venkatesh , and F.J. Doyle , "Multiple feedback loop design in the tryptophan regulatory network of Escherichia coli suggests a paradigm for robust regulation of processes in series", Journal of the Royal Society Interface , 3 , 383-391, (2006)
- N. U. Padhiyar, A. Gupta, A. Gautam, S. Bhartiya, F.J. Doyle III, S. Gaikwad and S. Dash, "Nonlinear inferential multi-rate control of kappa number at multiple locations in a continuous pulp digester" Journal of Process Control, 16, 1037-1053 (2006).
- A. Ruhela, M. Verma, J.S. Edwards, P.J. Bhat, S. Bhartiya , K.V. Venkatesh, "Autoregulation of regulatory proteins is key for dynamic operation of GAL switch in Saccharomyces cerevisiae ", FEBS Letters , 576 , 119-126, (2004).
- S. Bhartiya, P. Dufour and F.J. Doyle III , "Fundamental thermal-hydraulic continuous pulp digester model with grade transition", AIChE Journal , 49 , 411-425 (2003).

R. D. Gudi

B.Tech., I.I.T., Bombay, 1985.
Ph.D., University of Alberta, 1995.
ravindra@che.iitb.ac.in

Control Relevant Identification, Non Linear Identification, Scheduling and decision support, Fault Classification and Accommodation, Optimal Control of Fermentation Processes

Control relevant identification:
The research in this area is focused on building restricted complexity models for complex nonlinear processes, with a view to achieve desired closed loop performance. Methods related to generalized frequency response were analyzed and different model reduction strategies were proposed.

Nonlinear Identification:
Nonlinear structure identification as well as clustering and classification strategies were explored towards nonlinear identification. Properties of multivariate algorithms such as PCA and PLS were exploited to present some new results in recursive model identification for nonlinear processes.

Scheduling and Decision Support:
Issues related to vertical problemdecomposition to solve multiple horizon problems in reactive scheduling were considered. Disturbance / Fault Accommodation: Faults in operating process plants bring in their own signatures in terms of the patterns in the operating data. Clustering / classifying techniques were used to characterize the abnormal / aberrant operation separately from the normal operating region.

Optimal Control of Fermentation Processes:
Integrating design and control issues using stochastic optimization techniques have been the focus of some of our recent work in this area.

Selected Publications:

- Munawar S. A, Bhushan M., Gudi R.D, and Belliappa A. M., "Cyclic Scheduling of Continous Multiproduct Plants", To appear in *Industrial* and *Engineering Chemistry Research,* (2003).
- Meel A, Venkat A. and Gudi R. D., "Disturbance Classification and Rejection using Pattern Recognition methods", *Industrial and Engineering Chemistry Research*, **42** 3321-3333, (2003).
- Vijaysai P., Gudi R. D., and Lakshminarayanan S., "A New Recursive PLS approach for Dynamic Model Identification on Demand", *Industrial And Engineering Chemistry Research,* **42**, 540-554, (2003).

Sameer Jadhav

B.Tech. Chemical Engg., LIT, Nagpur University, 1995
M.Tech. Chemical Engg., IIT Kanpur, 1998
Ph.D. Chemical and Biomolecular Engg., Johns Hopkins University, 2004
srjadhav@che.iitb.ac.in

Cellular mechanics, Biomaterials, Tissue engineering, Modeling and simulation of biological processes

Cell adhesion and motility
Our goal is to elucidate the role of molecular interactions and cellular mechanics in cell adhesion, spreading and migration pertinent to vascular pathological processes such as thrombosis, inflammation and cancer metastasis.

Cell-biomaterial interactions
We are interested in understanding and controlling cellular interactions with synthetic biomaterials for potential applications in targeted drug delivery and tissue engineering.

Modeling and simulation of cell dynamics
We are developing predictive models for computer simulation of physiological and pathological processes involving cell adhesion, spreading and migration.

Selected Publications:

- S Jadhav, KY Chan, K Konstantopoulos, CD Eggleton, "Shear modulation of intercellular contact area between two deformable cells colliding under flow", J Biomech. 2007, 40(13): 2891-2897.
- S Jadhav, CD Eggleton, K Konstantopoulos, "Mathematical modeling of cell adhesion in shear flow pertinent to inflammation and cancer metastasis", Invited Review in Curr Pharm Des. 2007, 13(15):1511-26.
- S Jadhav, CD Eggleton, K Konstantopoulos, "A 3-D computational model predicts that cell deformation affects selectin-mediated leukocyte rolling" Biophys J. 2005 88(1):96-104.
- KC Ahn, AJ Jun, P Pawar, S Jadhav, OJT McCarty, K Konstantopoulos, "Preferential binding of platelets to monocytes over neutrophils under flow", Biochem Biophys Res Commun. 2005, 329(1):345-55.
- W Hanley, OJT McCarty , S Jadhav, Y Tseng, D Wirtz, K Konstantopoulos, "Single molecule characterization of P-selectin/ligand binding", J Biol Chem. 2003, 278(12):10556-61.

V. A. Juvekar

B. Chem. Engg., Bombay University, Bombay, 1970.
Ph.D., (Tech), Bombay University, Bombay, 1976.
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Adsorption and Ion exchange, Interfacial Engineering, Heterogeneous Reaction Engineering, Electrochemical Engineering

Adsorption
Work in collaboration with M/s Unilever Industries Ltd. on development of mathematical model for dynamics of adsorption of polymer at solid-liquid interface with the aim to develop more efficient anti-redeposition and soil-release agents

Ion-exchange
Study of dynamics of ion-exchange in resins with a view to understand the interplay of pore diffusion, electrical field at the charged pore surface and adsorption/disorption of ions

Interfacial Engineering
Studying various aspects of liquid-liquid interfaces. These include coalescence, interfacial reactions and microemulsion. One of the important reaction under study is aromatic nitration

Heterogeneous Reaction Engg.
Studies include reactive distillation, Friedel-Crafts alkylation and transalkylation, phase transfer catalysis, ion-exchange catalysis, liquid emulsion membranes etc.

Electrochemical engineering
Studies include bipolar electrolysis, structure and dynamics of double layers at high potentials and high frequency.

Selected Publications:

- Austine, J., Mohite L. V. and Juvekar, V. A., "An algorithm for simulating equilibrium adsorption characteristics of branched copolymer chains at solid-liquid interface", Macromolecular Theory and Simulations, 16, 3283-3295 (2007).
- Juvekar, V. A., Joshi, A. A., and Thoakar, R., "Enhancement of gas absorption by sparingly soluble fine particles reacting instantaneously with the dissolved gas: A cell model", Industrial and Engineering Chemistry Research, 46, 3283-3295 (2007).
- Austine, J. and Juvekar, V. A., "Prediction of energy of interaction among tethered polymer chains confined between two parallel plates", Macromolecules, 38, 3961-3972 (2005).
- Pattanayek, S. K. and Juvekar, V. A., "Adsorption of polymer from solution to solid surface: Effect of polydispersity", Macromolecules, 36, 956-960 (2003).
- Pattanayek, S. K. and Juvekar, V. A., "Prediction of adsorption of nonionic polymers from aqueous solutions to solid surfaces", Macromolecules,35, 9574-9580 (2002).

D. V. Khakhar

B.Tech., I.I.T., Delhi, 1981.
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Granular Flow & Mixing, Fluid Mixing, Chaotic Advection, Computational Fluid Dynamics, Polymerization of Rodlike Polymers, Polyurethane Foams

Granular flow and mixing:
Are of considerable importance for a large number of industrial applications (mixing of pharmaceuticals, cement manufacture) yet they are poorly understood. One of the complicating factors is simultaneous segregation due to differences in particle characteristics. Our work is focused on simple prototype mixers (rotating cylinders) to gain an insight into the fundamental physics. An application area of our interest is calcination and clinker formation in rotary kilns.

Fluid mixing:
Particularly of viscous liquids and pastes is a difficult operation. Chaotic advection greatly aids the process. We are using computational fluid dynamics and the tools of non-linear dynamics tomixing in systems of complex geometry.

Rodlike polymers:
can be spun into ultra high strength fibres (e.g. Kevlar) which find application in the manufacture of tyre cord, composites and bullet-proof fabrics. We are investigating the effect of orienting fields applied during polymerization on the kinetics and polymer formed.

Selected Publications:

- G. O. Fountain, D. V. Khakhar and J. M. Ottino, Visualization of three-dimensional chaos, *Science*, **281**, 683-686, (1998).
- A. Agge, S. Jain and D. V. Khakhar, Acceleration of polymerization of rodlike molecules by flow, *J. Am. Chem Soc.*,**122**,10910-10913 (2000).
- A. V. Orpe, and D. V. Khakhar, Scaling relations for granular flow in quasi-two-dimensional rotating cylinders, *Phys. Rev*. E, **64**, 031302 (2001).
- D. V. Khakhar, A. V. Orpe, P. Andresand J. M. Ottino, Heap formation in quasi 2d flows, *J. Fluid Mech*., **441**, 255-264, (2001).
- D. V. Khakhar, A. V. Orpe and S. K. Hajra, Segregation of granular materials in rotating cylinders, *Physica* A, **318**, 129-136, (2003).

K. C. Khilar

B.Tech., I.I.T., Kharagpur, 1975.
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Ph.D., University of Michigan, 1981.
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Nanoparticles and Liquid Nanocomposites, Colloids and Interface Science and Engineering, Transport in Porous Media

Nanoparticles: Our group has been working on the preparation of nanoparticles of metals, metal salts, metal oxides and semiconductor nanoparticles using water-in-oil microemulsions. We have been studying some of the important scientific and engineering issues both experimentally and theoretically. We are also currently studying the formation of nanoclusters from precursor solutions.

Liquid Nanocomposites: Our group has been working to develop superhydrophobic surface coatings based on both chemical and physical modifications on the surface.

Foams: Our group in the past has done some amount of work on liquid foams addressing both generation and stability issues. Currently we are working on the technology and modeling of metal foams.

Contaminants Transport in Porous Media: several years, customized simulators have been configured by my group in CAD Centre for Ammonia and Urea Processes based on rigorous mathematical models developed in-house for several plants in India. Efforts are continuing to enhance and strengthen the capabilities of these simulators.

Selected Publications :

- Book: Kartic C. Khilar and H.S. Fogler, "Migration of Fines in Porous Media", (Theory and Applications of Transport in Porous Media Series) Kluwer Academic Publishers, Dordrecht, The Netherlands, 1998.
- "Chracterization of Nanosized CdS-Ag2S Core-Shell Nanoparticles using XPS technique" Colloid and Surfaces A- Physicochemical and Engineering Aspects, 293 p.5-12 (2007) (with G. hota and S.B. Idage).
- "A Mean Phi Model for Pressure filtration of Fine and Colloidal Suspensions" Canadian Journal of Chemical Engineering, 84(1), p.83-93 (2006). (with S. Raha, Pradip and P.C. Kapur)
- "Synthesis of CdS-Ag2S Core-Shell/Composite Nanoparticles using AOT/n-Heptane/Water Microemulsions" Colloids and Surfaces A, Physicochemical and Engineering Aspects 232, p.119-127 (2004) (with G. Hota and S. Jain).
- "Modeling Nanoparticles Formation by Mixing of Two Reactive . Microemulsions" AIChE J. 50, P.1556-1567,(2004).

Mani Bhushan

B.Tech., I.I.T., Bombay, 1983.
Ph.D., I.I.T. Bombay, 1987.
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Fault Detection and Diagnosis, Sensor Network Design, Optimal Alarm Management, Planning and Scheduling in Process Plant, Process Safety Analysis

Measurement System Design: Development of techniques for designing measurement systems for meeting various objectives under specified constraints. Design includes selection of measurement variables, selection of sensors and their sampling frequencies. Objectives and constraints are related to fault-diagnosability, reliability, precision, accuracy, cost, etc.

Fault Diagnosis: Development and use of qualitative trend analysis, support vector machines and Fisher discriminant analysis based techniques for Fault Detection and Diagnosis mainly for batch processes, integration of qualitative data-based and quantitative model-based techniques for performing efficient FDD.

Alarm Management: Design of a systematic cost-based, multivariate alarm management framework that includes optimal strategies for alarm generation as well as alarm interpretation.

Filtering for State Estimation: Use of sampling based techniques such as unscented kalman filtering, particle filtering for state estimation of dynamic, nonlinear, multirate processes.

Other interests: Process safety analysis, modeling and analysis of discrete event systems, positive matrix factorization techniques for pollution source identification, modeling, monitoring and optimization of fermentation process.

Selected Publications

- M. Bhushan, S. Narasimhan and R. Raghunathan, "Robust sensor network design for fault diagnosis", Comp. & Chem. Engg., 32, 1067-1084, 2008.
- P. R. Kotecha, M. Bhushan, R. D. Gudi and M. K. Keshari, "A duality based framework for integrating reliability and precision for sensor network design", J. of Process Contr., 18, 189-201, 2008.
- S.C.Kadu, M. Bhushan and R. D. Gudi, "Optimal sensor network design for multirate systems", J. of Process Contr.,doi:10.1016/j.jprocont.2007.10.002, 2007.
- P. R. Kotecha, M. Bhushan and R. D. Gudi, "Constraint Programming Based Robust Sensor Network Design", Ind. Eng. Chem. Res., 46, 5985-5999, 2007.

Sanjay Mahajani

B.Chem., Mumbai University (UICT), 1989.
M. Tech. I.I.T., Bombay, 1992.
Ph.D., Mumbai University (UICT), 1996.
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Reaction Engineering and Catalysis, Multifunctional Reactors: Reactive Distillation, Reactive chromatography, Energy: Coal gasification, Biofuels, Fischer-Tropsch Synthesis, Computer Aided Design and Simulations, Computational Fluid Dynamics (CFD)

Reaction Engineering, Catalysis and Multifuctional Reactors: Studies in reaction kinetics of both catalysed/ uncatalysed homogeneous and heterogeneous reactions. Catalysis with solid acid catalysts like ion exchange resins, zeolites etc. for liquid phase organic reactions. Reactions in supercritical media. Experimental and theoretical investigations to check the feasibility of reactive adsorption (chromatography), reactive distillation and extractive reactions for industrially important processes.

Energy: Coal gasification, Biofuels, Fischer-Tropsch Synthesis: Underground Coal Gasification, Process and catalyst development studies in synthesis of biodiesel, Kinetics and reactor engineering for Fischer Tropsch Synthesis.

Computer Aided Design and Simulations: Conceptual Design of distillation and reaction systems, application of residue curve maps and attainable region concepts for reactive separation, Steady state and dynamic simulation of complex reaction systems e.g. reactive distillation, simulated moving bed reactors, Non-linear dynamic effects and Optimization.

Computational Fluid Dynamics: Studies on influence of flow patterns on the reactor performance. Determination of velocity field, power in agitated vessels. Compartment modeling based on residence time distribution for non-conventional reactors (e.g. underground coal gasification, mixer-settlers).

Selected Publications:

- Mahajani S. M., Kolah A. K. and Sharma M. M., Extractive Reactions with Cationic Exchange Resins as Catalysts: Acetalization of Aldehyde with Alcohols, React. Funct. Polym., 28, 1995, 29-38.
- Kolah A. K., Mahajani S. M. and Sharma M. M., Acetalization of Formaldehyde with Methanol in Batch and Continuous Distillation Column Reactors, Ind. Eng. Chem. Res., 35, 1996, 3707-3720.
- Mahajani S. M. and Kolah A. K., Some Design Aspects of Reactive Distillation Columns (RDC), Ind. Eng. Chem. Res., 36, 1996, 4587-4596.
- Mahajani S. M. and Sharma M. M., Reaction of Glyoxal with Aliphatic Alcohols Using Cationic Exchange Resins as Catalysts, Org. Proc. Res. Dev., 1, 1997, 97-105.
- Singh K. K., Mahajani S. M., Shenoy K. T., Ghosh S. K., CFD Modeling of Pump-Mix Action in Continuous Flow Stirred Tank, AIChE J., 54(1), 2008.

R. K. Malik

B.Sc., Engg., Kanpur University, 1970.
M.Tech., I.I.T., Kanpur, 1973.
Ph.D., University of Wisconsin, Madison, 1979.
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Chemical Process Simulation, Process Design & Optimization, Energyanalysis & Process Integration, Process Intensification, Multistage Separation Processes

Development of efficient strategies to model and simulate various petroleum processes (primarily, staged separation processes, and processes having reactive systems) has been of great interest to me. Recent research done by my group has looked into the phenomena of solution multiplicity in distillation columns. Energy analysis of distillation columns for process integration; planning & optimal operation in refineries; and resource optimization (water management) have been the subjects of my recent collaborative research with Prof. U.V. Shenoy. Over the past several years, customized simulators have been configured by my group in CAD Centre for Ammonia and Urea Processes based on rigorous mathematical models developed in-house for several plants in India. Efforts are continuing to enhance and strengthen the capabilities of these simulators.

Selected Publications:

- Malik R. K., and R. R. Hughes, "Optimal design of flexible chemical processes", Computers and Chemical Engineering, **3**, (1979).
- Malik, R. K., "Modeling and Simulation as Tools for Process Optimization and its Applications in fertilizer Plants", Fertilizer News, May 1991, **36** (5).
- Bandyopadhyay S., Malik, R. K., and Shenoy U. V., "Temperature enthalpy curve for energy targeting of distillation columns", Computers and Chemical *Engineering*, **22**(12), 1713-1744 (1998).
- Bandyopadhyay S., Malik R. K., and Shenoy U. V., Invariant rectifying-stripping minimum energy and feed location in distillation, Computers and *Chemical Engineering*, **23**(7), 1109-1124 (1999).
- Dalal N. M. and Ranjan K. Malik, Solution Multiplicity in Multicomponent Distillation - A Computational Study, *ESCAPE-13*, Elsevier Science (2003).

A. Mehra

B.Tech., I.I.T., Kanpur, 1983.
Ph.D. (Tech.), Bombay University, 1987.
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Heterogeneous reactions, Mass transfer, Surfactant systems, Multiphase Precipitations, Nanoparticles.

Multiphase Reaction Engineering:
Heterogeneous reactions controlled by diffusional factors pose novel problems when conducted in microheterogeneous media such as emulsions, slurries and other types of surfactant based systems. The diffusion-reaction characteristics in such media are being investigated. The work includes looking at basic mass transfer examining reactant particle size related effects in slurry absorbers / precipitators etc.

Nanoparticles:
The use of micelles and microemulsions to produce nanoparticles of inorganic salts (eg. silver chloride, cadmium sulfide) provides a novel route to the manufacture of these nanomaterials. The mathematical modeling of the formation of these particles, including the case of complex/composite particles is of interest. Also, of interest is the formation of these particles in multiphase systems (eg. nanoparticles of calcium carbonate in gas-slurry-micellar systems)

Demulsification:
The demulsification of surfactant stabilized emulsions is being studied in simple shear flows in order to obtain information about the transient evolution of droplet size distributions as a function of the shearing rate, surfactant concentrations and dispersed phase hold up.

Selected Publications:

- Jain, R. and Mehra, A., 2004, ``Monte Carlo Models for Nanoparticle Formation in Two Microemulsion Systems", Langmuir, 20, 6507-6513.
- Nandi, A., Mehra, A. and Khakhar, D.V., 2006, "Coalescence in a Surfactant-less Emulsion under Simple Shear Flow'', AIChE J, 52, 885-894.
- Shukla, D. and Mehra, A., 2006, "Modeling the Formation of Shell in Core-Shell Nanocrystals in Reverse Micellar Systems'', Langmuir, 22-23, 9500-9506.
- Sugih, A.K. and Shukla, D. and Heeres, H.J. and Mehra, A., 2007, "CaCO3 Nanoparticle Synthesis by Carbonation of Lime Solution in Microemulsion Systems, Nanotechnology, 18, 035607
- Kakaraniya, S.J., Gupta, A. and Mehra, A., 2007, ``Reactive Precipitation in Gas-Slurry Systems: The CO2-Ca(OH)2-CaCO3 System'', Ind. Eng. Chem. Res., 46, 3170-3179.

S. Mehra

Integrated M. Tech (Dual Degree), Biochemical Engineering and Biotechnology, IIT Delhi, 1999.
Ph.D., Chemical Engineering, University of Minnesota, 2005.
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Systems biology and functional genomics, Metabolic engineering, High-throughput data analysis, Modeling of genetic regulatory networks.

Systems Biology: A system under investigation involves the cellular networks responsible for resistance to commonly used antibiotics and drugs to build a global map of resistance mechanisms in Streptomyces coelicolor. In another multi-institutional project, we are examining the regulatory networks involved in stress response and pathogenesis in Mycobacterium species. A multidisciplinary approach using high-throughput experimental techniques such as whole genome expression profiling using microarrays combined with computational tools is being used to decipher these networks.

Cell Culture Engineering: The demand for recombinant therapeutic proteins produced in animal cell lines has increased dramatically in recent years. In this project we are investigating the biology of mammalian cell lines under production conditions and subsequently implement different cell engineering approaches to improve their productivity.

Mathematical Modeling of Genetic Networks: Signaling molecules produced by bacteria for inter-cellular communication play an important role in many biological processes such as the dissemination of antibiotic resistance by enterococci and initiation of antibiotic synthesis in Streptomyces. We are using deterministic and stochastic models coupled with cell population balance models to understand the dynamics of such systems.

Selected Publications

- Charaniya, S., S. Mehra, S., Lian, W., Jayapal, K. P., Karypis, G., and Hu, W.-S, "Transcriptome dynamics-based operon prediction and verification in Streptomyces coelicolor." Nucleic Acids Res., 35(21), 7222-36, 2007.
- Mehra, S., Lian, W., Jayapal K., Charaniya S., Sherman, D., and Hu, W.-S, A Framework to Analyze Multiple Time-Series Data: A Case Study with Streptomyces coelicolor, J. Ind. Microbiol Biotechnol, 33(2), 159-72, 2005.
- Mehra, S., and Hu, W.-S, A Kinetic Model of Real-Time Polymerase Chain Reaction, Biotechnol Bioeng, 91(7): 848-60, 2005.
- Mehra, S., Hu, W.-S., and Karypis, G., A Boolean Algorithm for Reconstructing the Structure of Regulatory Networks, Metab Eng, 6(4): 326 -39, 2004.

A. Misra

B.Tech., I.I.T., Kanpur, 1968.
M.S.,Tufts University, Medford, 1969.
M.S., Polymer Science & Engineering, University of Massachusetts, Amherst, 1971.
Ph.D., Polymer Science & Engineering, University of Massachusetts, Amherst, 1974.
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Engineering Polymers, Polymer Blends and Alloys, ThermoPlastic Composites, Nano-composites, Liquid Crystal Polymers and their Blends, Polymer Rheology and Processing, oriented Polymer Films, Incremental Drawing of Synthetic fibres and Polymer Product design.

Structure property correlations in polymer systems

The systems studied include polymer blends and alloys, semi-crystalline polymers, liquid crystalline polymers, self-reinforcing composites (blends of LCP and conventional polymers), and thermoplastic composites. The recent work on polymer blends and alloys using reactive processing offer opportunities for designing polymeric materials for engineering applications with attractive performance properties.

Poly(vinylidene fluoride) (PVDF) films:

The combination of stretching and poling in high electric fields of PVDF films induces a larger proportion of the desired b-phase crystallites and irreversible dipole reorientations imparting very good piezoelectric properties. The objective of this work is to enhance the understanding of the structural changes that take place on account of uniaxial orientation and electrical polarization and their correlation with performance properties.

Polymer - layered silicate nanocomposites:

The current work is focused on PET-clay nanocomposites using the melt-intercalation process. The special features of intercalation and exfoliation are being studied using characterization techniques like WAXD, FTIR, TEM and DSC. The aim is to develop materials for engineering and other applications.

Selected Publications:

- A.K. Mukhopadhyay, B. Dutta and A. Misra, Incremental Drawing of Polyethylene Terephthalate Partially Oriented Yard (PET-POY), *International Polymer Processing,* **5,** 32-36 (1990).
- M. Joshi, S.N. Maiti, R.K. Mittal and A. Misra, Studies on Short Glass Fibre Reinforced Polybutylene Terephthalate/ Polyolefin Alloys I: Mechanical Properties and their dependence on Fibre Length Distribution, Fibre Orientation and Interfacial Adhesion, *Polymer Composites,* **15,** 349 (1994).
- G. Sawhney, S. K. Gupta and A. Misra, Structure and Properties of Blends of a Thermotropic LCP with a Commercial Alloy of Nylon-6 and ABS, *J. Appl. Polym. Sci.,* **62,** 1395 (1996).

A. S. Moharir

B.Tech., Nagpur University, 1975.
Ph.D., I.I.T., Kanpur, 1980.
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Adsorption Separation, Reactor Modeling, Flowsheeting, Computer Aided Design and Engineering, Fluid Network Analysis, Transient Fluid Flow Analysis, Process Plant Engineering, Piping Engineering.

Adsorptive separations:
Research on adsorptive separations such as PSA, VSA, SMB, CCMB is being carried out. A generic object oriented modeling platform for SMB systems has been created and tested.

GRM (General Reactor Model):
GRM (General Reactor Model), an object oriented implementation of a reactor modeling system, which facilitates model development of single as well as multi-phase industrial reactor systems has been developed and delivered to a major technology licenser.

Integrated IT and CAD aids:
Research related to developing integrated IT and CAD aids to support technical feasibility studies, pilot plant data analysis and model building conceptual process design, detailed process design, detail engineering, operating optimization etc. Research has mainly been of applied nature. Continuing interest has been in adsorptive separations such as PSA, VSA, SMB, CCMB. A generic object oriented modeling platform for SMB systems has been created and tested. GRM (General Reactor Model), an object oriented implementation of a reactor modeling system, which facilitates model development of single as well as multi-phase industrial reactor systems has been developed and delivered to a major technology licenser.

Selected Publications:

- Rajasree R., Moharir A. S., Simulation based synthesis and optimization of pressure swing adsorption (PSA) processes; *Computers and Chemical Engineering*, **24**, (2000), 2493-2505.
- Moharir A. S., Shah S. S., Gudi R. D., Devereux B. M., Bussche K. V., Venimadhavan G., Generalized Reactor Model : An Object Oriented Approach to Reactor Modeling, *ESCAPE 11*: Denmark 2001.
- Jain S., Moharir A. S., Li P, Wozny G, Heuristics Design of Pressure Swing Adsorption: A Preliminary Study; *Separation and Purification Technology;* **33,** (2003), 25-43.

Kannan M. Moudgalya

B.Tech, I.I.T., Madras, June 1980.
Ph.D, Rice University, May 1985.
Master of Electrical Engineering, Rice University, May 1985.
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Control system design, digital control, process control. Differential algebraic systems, optimization. Modelling, simulation and control of automotive systems, esp. IC engines. Identification and control of computing systems. Educational methodologies. Development of educational material using Scilab.

Books:

- K. M. Moudgalya, "Digital Control", John Wiley & Sons, Chichester, UK, July 2007.
- M. C. Joshi and K. M. Moudgalya, "Optimization: Theory and Practice", Narosa Publishers, New Delhi, 2004, alpha-Interscience, London, 2004.

Selected Publications:

- A. M. Katariya, R. S. Kamath, K. M. Moudgalya and S. M. Mahajani, "Non-equilibrium stage modeling and non-linear dynamic effects in the synthesis of TAME by reactive distillation", Computers and Chemical Engineering, in print, 2008.
- J. Agrawal, K. M. Moudgalya and A. K. Pani, "Sliding motion of discontinuous dynamical systems described by semi-implicit index one differential algebraic equations", Chemical Engineering Science, Vol. 61, 4722-4731, 2006.
- K. M. Moudgalya, S. K. Singh, K. P. Madhavan and G. Jain, "A class of discontinuous dynamical systems IV. A laboratory air-water System", Chemical Engineering Science, Vol. 58, 3973-3983, 2003.
- K. M. Moudgalya and V. Ryali, "A class of discontinuous dynamical systems I. An ideal gas-liquid system", Chemical Engineering Science, Vol. 56, 3595-3609, 2001.
- S. Shah, K. M. Moudgalya and K. Ramamritham, "Feedback Control of Internet Applications involving the Tracking of Dynamic Data", 17th IFAC world congress, July 6-11, 2008, Seoul, Korea.
- K. M. Moudgalya, "Discrete time control: a first control course", Advances in control education, IFAC, Madrid, 21-23 June 2006.

M. Mukhopadhyay

B.Ch.E., Jadavpur University, Calcutta, 1963.
M.Tech., I.I.T., Kharagpur, 1965.
Ph.D., Ohio State University, Columbus, 1969.
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Thermodynamics, Supercritical Fluid Extraction, Processing with Supercritical Fluids, Production of Nanoparticles, Food Process Engineering and Cryogenics.

Our group is engaged in research in the following areas :

- Measurement of Thermodynamic and Phase equilibrium properties.
- Process design and simulation of distillation, extraction, and Supercritical fluid extraction.
- Supercritical extraction of natural products using process innovations.
- Thermodynamic modeling with new mixing rules for complex natural product systems.
- Mass transfer modeling of supercritical extraction and fractionation processes.
- Reaction kinetics in supercritical carbon dioxide medium with simultaneous phase separation.
- Development of Dense Carbon Dioxide Anti solvent Technology for purification and micronisation of phytochemicals and pharmaceuticals,
- Thermodynamic and mass transfer modeling, super saturation and nucleation kinetics for production of ultra-fine or nanoparticles.
- Sterilization, stabilization and preservation of food products using dense carbon dioxide.
- Design and development of SCFE plant for multiple products with innovative design features aimed at substantial cost reduction.

Selected Publications:

Books Authored:

- M. Mukhopadhyay, "Natural Extracts Using Supercritical Carbon Dioxide" CRC Press LLC, Florida (2000).
- M. Mukhopadhyay, "Phase Equilibrium in Solid - Liquid - Supercritical Fluid Systems Chapter-2 in Drug Delivery and Supercritical Fluid Technology", Marcel Dekker Inc. New York 2003.

Patents Granted:

- "Process for Supercritical Fluid CO2 Extraction of Fragrances (absolute or essential oils) from Jasmine flowers", Indian Patent # 183454 (72/Bom/96).
- "Process for Sequential Supercritical CO2 Extraction and Fractionation of Neem Oil Enriched with Azadirachtin from Neem kernels", Indian Patent # 182587 (428/BOM/97).

Journal publication:

- M. Mukhopadhyay, "Partial Molar Volume Reduction of Solvent For Solute Crystallization Using Carbon Dioxide as Antisolvent", *J. Supercritical Fluids,* **25**, No.3, 213-223, (2003).

Hemant Nanavati

B.Tech. I.I.T., Bombay, 1989.
M.S., Georgia Tech., Atlanta, 1992.
Ph.D., Georgia Tech., Atlanta, 1998.
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Polymer Physics: Network Elasticity, Structure-Property Relationships, Polymer Phase Transitions, Molecular Simulation, Coarse Graining of Polymer Melts, Biodegradable Polymers; Protein Structure Prediction

Polymer Structure-Property Relationships: The aim is to bridge the gap between information from the primary molecular structure and useful, applied properties. In the case of Elastomeric Polymer Networks (Crosslinked Network, Fiber Network and Thermoplastic Elastomer morphologies), our approach developed incorporates primary molecular structural aspects into the theoretical and computational formulations, leading to accurate and objective stress-strain-orientation relationships. Work is in progress on the computational and theoretical analysis of collapse transitions of co-polymers, and crystallization in polymers with additives. Ongoing work includes synthesis, processing and solid state polymerization for Value-Added Lactic Acid Biodegradable Polymers and their Nanocomposites.

Ongoing Research Includes:

ab initio Protein Structure Prediction; Coarse Graining and Primitive Path Analyses of Polymer Melts.

Selected Publications:

- Vimal Katiyar and Hemant Nanavati, "Polylactic acid-clay nanocomposites and process for preparing them", Indian Patent Application No. 677/MUM/2007.
- Vimal Katiyar and Hemant Nanavati, "Method for producing lactic acid polymers of high crystallinity and molecular weight", Indian Patent Application No. 678/MUM/2007.
- Vimal Katiyar and Hemant Nanavati, "Polylactic acid-clay nanocomposites by lactide polymerization in clays", Indian Patent Application No. 679/MUM/2007.
- Kapileswar Nayak, Sushanta Das and Hemant Nanavati*, "Elasticity and Photoelasticity Relationships of PET Fiber Networks by Molecular Simulations", J. Chem. Phys. 128, 014902, 2008
- Ashok Kumar Dasmahapatra, Hemant Nanavati, and Guruswamy Kumaraswamy, "Pathway to copolymer collapse in dilute solution: Uniform versus random distribution of comonomers", J. Chem. Phys., 127, 234901, 2007
- Ashok Kumar Dasmahapatra Guruswamy Kumaraswamy Hemant Nanavati, "Collapse Transition in Random Copolymer Solutions", Macromolecules, 39 (26), 9621 -9629, 2006.
- Gaurav Porwal, Swapnil Jain, S Dhilly Babu, Deepak Singh, Hemant Nanavati, Santosh Noronha, "Protein structure prediction aided by geometrical and probabilistic constraints", J Comput Chem. 12:1943, 2007.

S. Noronha

B.Tech., Chemical Engg., I.I.T. Madras, 1990.
Ph.D., University of Maryland, Baltimore County, 1996.
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Biochemical Engineering

Bioprocess development:
Development of recombinant routes for synthesis of chiral intermediates. Development of novel recombinant bacterial and fungal expression systems. Isolation of novel enzymes from filamentous fungi. Rational protein engineering for improved biocatalysis and sensitivity. Development of adaptive bioreactor process control techniques. Affinity purification of biologicals.

Systems Biology:
Experimental and computational investigations of Oxidative and metal stress response networks in E. coli and B. subtilis. Pathway and protein engineering for overproduction of fermentative metabolites.

Data analysis:
Application of pattern classification and computer-intensive methods for the following problems: Motif identification in genomes of parasites. Pattern identification in protein structures. Fault detection in process data. Ab initio and heuristic based protein structure prediction.

Selected Publications:

- L. Trinh, S. Noronha, M. Fannon and J. Shiloach. 2000. Recovery of mouse endostatin produced by Pichia pastoris using expanded bed adsorption. Bioseparation, 9: 223-230.
- S. Noronha, H. J. Yeh, T. F. Spande and J. Shiloach. 2000. Investigation of the TCA cycle and the glyoxylate shunt in Escherichia coli BL21 and JM109 using (13)C-NMR/MS. Biotechnol. Bioeng. 68(3): 316-327.
- S. Noronha, J. Kaufman and J. Shiloach. 1999. Use of Streamline chelating for capture and purification of poly-His-tagged recombinant proteins. Bioseparation, 8: 145-151.
- S. Noronha, L. W. Wagner, N. H. Matheson and J. Shiloach. 1999. Use of an ethanol sensor for feedback control of growth and expression of TBV25H in Saccharomyces cerevisiae. Biotechnol. Bioeng., 63: 285-289.

S. C. Patwardhan

B.Tech., I.T., B.H.U., 1986.
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Nonlinear Model Predictive Control, Linear and Nonlinear System Identification, Fault Tolerant Control Systems, Adaptive Control of Semi-batch Fermentation

Nonlinear Model Predictive Control: Development of discrete dynamic models suitable for formulating efficient predictive control strategies forcontrolling highly nonlinear systems; development of efficient methods for state estimation and control of nonlinear systems subject to stochastic unmeasured disturbances.

Identification of Linear and Nonlinear Multivariable Systems:
Identification of minimal order linear and nonlinear state space models of multivariable systems subject to unmeasured disturbances; para-meterization of state space models using generalized orthonormal basis filters (GOBF); estimation of time delays and multi-rate systems; on-line identification.

Fault Tolerant Control and Adaptive Scheme (FTCS):
Integration of on-line fault diagnosis and identification (FDI) with conventional and model predictive controllers; Developing FTCS for large scale plants and nonlinear systems.

Modeling and Optimal Control Semi-batch Processes: modeling batch / semi-batch processes from historical records of input - output data using artificial neural networks; computing optimal operating policy. Development of intelligent and adaptive control networks based on field-bus architecture.

Selected Publications:

- J. Prakash, S. C. Patwardhan, S. Narasimhan, "A Supervisory Approach to Fault Tolerant Control of Linear Multivariable Systems", *I & EC Res.*, **41**, 2270-2281, 2002.
- K. Kishore Kumar and Sachin C. Patwardhan, "Nonlinear Predictive Control of Systems Exhibiting Input Multiplicities Using Multi-Model Approach", *I & EC Res.*, **41,** 3186-3198, 2002.
- S.C. Patwardhan and K.P. Madhavan, "Nonlinear internal model control using quandratic models", *Comp. & Chem. Eng.,* **22**, 587, 1998.
- S.C. Patwardhan and K.P. Madhavan, "Improved Techniques for Development of Quandratic Perturbation Models", *I & EC Res.*, **35**, 4281, 1996
- S.C. Patwardhan and K.P. Madhavan, "Nonlinear predictive control using quadratic prediction models", *I & EC Res.,* **32,** 331, 1993.

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Environmental Engineering, Fluidization, Drying, Fluid Dynamics and Heat Transfer in Packed Beds

Photochemical Oxidation: The removal of toxic and hazardous organic compounds present in industrial waste water effluents becomes often difficult and expensive when treated with conventional chemical oxidants. Further, the conventional transfer technologies simply transfer the pollutants from one phase to other phase, thus not really addressing the disposal of the pollutant. Advanced Oxidation Processes (AOPs) can be used to address these problems. These processes can be operated at near ambient temperature and atmospheric pressure, which involve generation of highly active hydroxyl radicals in the presence of UV light or using Fenton reagents. The associated rate of reaction is many folds higher as compared to the conventional oxidants. The current research is focused on degradation of organic pollutants by homogeneous H2O2 – UV, heterogeneous TiO2 catalyzed UV, and Fenton and photo Fenton processes.

Fluidization: The research is focused on bubbling and circulating fluidized beds. In bubbling beds, hydro chlorination of silicon to produce trichlorosilane is modeled taking into account bubble dynamics on the process. In circulating fluidized beds, wall to bed heat transfer, intermixing of gas streams, and solid circulation are being studied.

Selected Publications:

- B. Bhattacharya, D. Sathiyamoorthy, V. Govardhana Rao and S.P. Mahajan, (2000) "Critical bed heights for solid circulation in a compartmented gas fluidized bed", Chem. Eng. Technol., 23, 1087-1098.
- V. Govardhana Rao, S. Mande and V.V.N. Kishore, (2001) "Study of drying characteristics of large cardamom", Biomass and Bioenergy, 20, 37-43.
- A.K. Saxena, V. Venkat Raj and V. Govardhana Rao, (2001) "Experimental studies on rewetting of hot vertical annular channel", Nuclear Engineering and Design, 208, 283-303.
- Krupesh Sheth and V. Govardhana Rao, "Photochemical oxidation of phenol using UV-TiO2 system in an annular fluidized bed reactor – A comparative study of synergy effects of impregnation of TiO2 on inorganic adsorbents", CHEMCON–2005, Organized by IIChE at New Delhi, Dec. 2005.

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Risk-based maintenance optimization, Detergency processes, Super-hydrophobicity, Supercritical fluid-based micronization.

Risk-based maintenance optimization: Models for Risk-based management of maintenance of chemical process are being developed. They include approaches that involve stochastic modeling of failure processes, fuzzy logic for multi-criteria decision-making for maintenance programs for process plants. Traditional identification methods such as FMEA are incorporated in the maintenance models

Detergency process: The phenomenon of oily soil removal from fabric surfaces during detergency process is being studied experimentally and theoretically. The theoretical approach aims at predicting the conditions for dynamic rollup and eventual detachment of the oily soil droplets from the solid fabric surface.

Supercritical fluid extraction: Supercritical fluid-based micronization is being studied for a number of pharmaceutical active agents for production of sub-micronic particles. The work involves evolving techniques of micronization considering the specific affinity or antipathy to supercritical carbon dioxide.

Ion-exchange Based Purification of Surfactants: The work involves employing a lumped parameter model to capture the complex double-layer effects that play a role in transport of charged species within the pores of resin particles.

Super-Hydrophobic Surfaces: Experimental work on the development of super-hydrophobic surfaces using a combination of polymeric substances ans nano-particles (embedded) is underway.

Selected Publications:

- Roy, S., Mehra, A. and Bhowmick, D., "Prediction of Solubility of Nonpolar Gases in Micellar Solutions of Ionic Surfactants'', J. Coll. Inter. Sci., 196, 53-61 (1997).
- Hasnat, A. and Roy, S., "Intensification of Instantaneous Heterogeneous Reactions by Simple Inert Electrolytes and Ionic Micelles", AIChE J., 44, 656(1998).
- Hasnat, A. and Roy, S., "Microphase Enhanced Reactions: Simultaneous Effects of Ion-Coupling and Counterion Binding", I & EC Res, 38, 4571(1999).
- Sen, A., Roy, S., and Juvekar, V. A., "Effect of Structure on Solution and Interfacial Properties of Sodium Polystyrene Sulfonate", Polym. Int., 56, 167 (2007).

H. S. Shankar

B.Tech., (Hons), I.I.T., Kharagpur, 1969.
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Multiphase Reaction Engineering, Biochemical Engineering, Process Simulation, Analysis & Synthesis in areas of energy, environment, Food, pharmaceuticals and Natural products processing

Hydrolysis of vegetable oils (1978-85):
Vegetable oils are hydrolyzed to produce fatty acids and glycerol; this work via a model synthesizes 35 years laboratory and plant data on the subject; fieldwork indicates that the model provides a powerful tool for design, operation and retrofitting. Early work was concerned with catalytic reaction engineering.

Gas solid reaction engineering (1984-92):
Development of continuous reactor-regenerator lab facility models to describe the system (2,3) takes place. Related work in the area of transport reactors and solid-solid reactions has revealed several new features. Theoretical and experimental studies in ipenicillin G hydrolysis with immobilized enzymes have revealed interesting features yielding significant benefits to process industry.

Ecological Engineering (1990 onwards):
The science and the art of combining organics, inorganics and life forms to derive value addition is being developed. The process engages an ecology consisting of soil, plants and select soil micro & macro-organisms including geophagous earthworms. The technology known as Soil Biotechnology (SBT) has been patented in India and USA. SBT has a very large clientele in city farming , animal husbandry, agriculture, wasteland development, agro-industrial waste processing.

Selected Publications:

- Patil T. A., Butala D. N., Namdev P. D., Shankar H. S. "Thermal hydrolysis of vegetable oils Part I, II, III", *IEC Res* **27,** 727 - Hydrolysis of vegetable oils Part I, II, III", *IEC Res* **27**, 727-743 (1988).
- Joshi P. A., Chidambaram M., Shankar H. S. "Non Catalytic Reactions incirculating fluidised beds", *Ed. Basu.P, Pergaman Press, NewYork,* 423-429 (1986).
- Kumar R., Suresh A. K., Shankar H. S., "Kinetics and reaction engineering of Penicillin G hydrolysis", *J. Chem. Tech. Biotechnol,* **66,** 243-250 (1996).
- Patnaik B. R., Bhawalkar U. S., Gupta A., Shankar H. S., "Residence Time Distribution in Soil Filters", *Waste Environment Research* (2003) in Press.

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Reaction Engineering, Multiphase systems, Biochemical Engineering, Interfacial polycondensation, Liquid phase organic oxidations.

Mass transfer with chemical reaction:
Intensification of mass transfer processes, mass transfer theories, concentrated dispersions, interfacial reactions.

Biochemical Engineering:
Enzymatic reaction kinetics, enzyme action in heterogeneous media. Fermentation technology - kinetic modelling, operating strategies for productivity enhancement, simultaneous saccharification and fermentation of starchy substrates, novel techniques for oxygen supply to viscous aerobic fermentations. Applications to lactic acid , diacetyl and xanthan gum fermentations.

Polymer reaction engineering:
Interfacial polycondensation - kinetic modelling, correlation between reaction rate, polymer structure and performance in applications such as controlled release microcapsules and thin film composite membranes.

Liquid phase organic oxidations:
Kinetics and reaction engineering of catalyzed and uncatalyzed autoxidations

Selected Publications:

- S.K. Karode, S.S. Kulkarni, A.K. Suresh and R.A. Mashelkar, "New insights into kinetics and thermodynamics of interfacial polymerization", *Chem. Eng. Sci.*, **53**, 2649-2663 (1998).
- A. K. Suresh, M. M. Sharma and T. Sridhar, "Engineering aspects of industrial liquid phase air oxidation of hydrocarbons", *I & EC Research*, **39**(11), 3958-3997 (2000).

Anurag Mehra, P. Basu and A. K. Suresh, "Reactive Dissolution of Particle Clusters", *I&EC Research,* **40,** 4050-4057 (2001).

A. K. Suresh and S. Bhalerao, "Rate Intensification of Mass Transfer Process using Ferrofluids", *Ind. J. Pure & Appl. Phys.*, **40**, 172-184 (2001).

S. Sahoo, R. K. Verma, A. K. Suresh, K. K. Rao and G. K. Suraishkumar, Micro-level and genetic responses of Bacillus subtilis to shear stress, Biotech Progress, **19,** 1689(2003).

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Rapid flows of Granular Materials, Dynamics of Dilute Polymer Solutions, Biomolecules in Microfluidic Devices, Flow of Liquid Crystals

Microfludic drug encapsulation in vesicles:
This project is part of a larger project to develop a microfludic device for synthesising vesicles for targeted drug delivery. In this part of the project, we aim to study few designs of a microfluidic device that can simultaneously synthesize vesicles and encapsulate drug inside it.

Viscoelastic Liquid Droplets:
The dynamics of deformation of a liquid drop as it forms in a cylindrical faucet or when it impacts a solid surface, has significant consequences in several applications such as: atomisation and sprays, ink jet printing, deposition of aerosols in lungs, delivery and deposition of agrochemicals, plasma spraying etc. This study aims to model and simulate drop dynamics through a combination of molecular simulations and continuum methods.

Dynamics of DNA in Microfluidic Devices: Emerging technologies for single bio-macromolecule (such as DNA and protein) analysis in micro- and nano-meter devices have generated interest in understanding the dynamics of these macromolecules in confined geometries. This study focuses on developing simulation algorithms to better describe the dynamics of DNA in microchannel flows.

Selected Publications:

- Sunthar, P. and J. R. Prakash (2006) Dynamic scaling in dilute polymer solutions: The importance of dynamic correlations. Europhys. Lett. 75 77-83.
- Sunthar, P., Nguyen, D. A., Dubbelboer, R., Prakash, J. R., and Sridhar, T. (2005) Measurement and prediction of the elongational stress growth in a dilute solution of DNA molecules Macromolecules 38, 10200-10209.
- Sunthar, P. and Prakash, J. R. (2005) Prediction of the chain length effects in elongational flows of dilute polymer solutions by successive fine graining. ANZIAM J. 46 C320-C335.
- Sunthar, P. and Prakash, J. R. (2005) Parameter free prediction of DNA conformations in elongational flow by successive fine graining. Macromolecules 38 617-640.

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Hydrodynamic and Electrohydrodynamic stability, Nanoparticle synthesis, Polymer and surfactant Physics and Rheology, Colloidal systems

Nanoparticle synthesis: We aim to undertake several studies to clearly identify factors affecting size, shape and distribution for nanoparticles and identify parameters crucial in large scale synthesis.

Colloidal Physics: We investigate the deformation of drops and vesicles in electrolyte solutions, by linear and nonlinear stability analysis supported by numerical calculations.

Polymer Physics and Nano-machines: We try to construct self propelled configurations of DNA using the asymmetric hamiltonian of a semiflexible polymer and driven by the ratchet effect. This can be a potential nanomachine which can selectively deliver drugs, genes and other cargo inside a cell in advanced medical therapy.

Hydrodynamic and Electrohydro-dynamic stability: We study the effect of oscillatory shear, which represents most biological flows, on the instabilities generated due to flow over soft materials. Electro hydro dynamics and electrokinetics find extensive use in Lithography and in colloidal systems respectively. Better understanding of these systems can lead to tighter control of the product quality in the field of nanotechnology and microfluidics.

Selecetd Publications:

- Thaokar, RM " Hydrodynamic interaction between two tori", Accepted EPJB
  Thaokar RM " Brownian dynamics of a rotating torus", Accepted Colloids and surfaces A
- Thaokar RM, Schiessel H and Kulic I M," Hydrodynamics of a rotating torus", accepted, EPJB , 2007.
- Juvekar, VA, Joshi, A and Thaokar, RM, Enhancement of gas absorption by sparingly soluble fine particles reacting instantaneously with a dissolved gas: A cell model, Industrial engineering and Chemistry, 45(10), 3283 - 3295, 2007.
- Igor M. Kulic, H. Mohrbach, R. Thaokar, H. Schiessel, "Equation of state of looped DNA", Physical Review E, Phys. Rev. E 75, 011913-1-23, 2007.
- I. M. Kulic, R. Thaokar,and H. Schiessel, A DNA ring acting as a thermal ratchet, J. Phys.: Condens. Matter 17, S3965-S3978 ,2005
- Igor M. Kulic, H. Mohrbach, V. Lobaskin, R. Thaokar, H. Schiessel, "Apparent Persistence Length Renormalization of Bent DNA", Physical Review E,72,041905-1-5, 2005

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Low Reynolds number hydrodynamics, Colloids and interface science

Our research group works on problems in the broad areas of fluid mechanics and colloids and interface science. In fluid mechanics, we have been investigating thin film flows of non-Newtonian liquids and stability of thin liquid sheets. In the colloids area, we have been investigating the film formation and cracking phenomenon in drying colloidal films. Major fact of promoting the recent investigation in this subject is the need to substitute the widely used coating formulations containing volatile organic compounds with environment-friendly water based dispersions. Here, we would like to know the effect of various parameters such as inter-particle potentials, pigment characteristics, polymer particle size, polymer modulus on the film's microstructure and its final mechanical properties.

Recently, we have also been involved in investigating the response of micro-organisms to nutritional gradients in microfluidic devices. Our research approach utlizes both experiments and computations to understand the fundamental issues in a wide variety of applications ranging from paints and coatings to bacterial mobility.

Selected Publications:

- S. Bajpai and M. Tirumkudulu, "An experimental study of impulsively started turbulent axisymmetric jets", EPJ B, 61,293-297 (2008)
- P K Jha and M Tirumkudulu, "Measurement of tack of Newtonian liquids on porous substrates", 19, 1 (2007)
- K B Singh and M Tirumkudulu, "Cracking in drying colloidal films", Phys Rev Lett, 98, 218302 (2007)
- M Tirumkudulu and W B Russel, "Cracking in drying latex films", Langmuir, 21(11), 4938 (2005)

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Atmospheric aerosols and climate, Aerosol source identification, Nanoparticle aerosol drug delivery

Aerosols and climate: Recent observational campaigns points to large spatial and temporal variability in surface and elevated aerosols over the Indian subcontinent, along with significant surface cooling and atmospheric heating. General circulation and chemical transport models with aerosol emission inventories developed in our group are being used to investigate aerosol effects on regional radiative forcing and climate.

Aerosol source identification: Aerosol sources and transport pathways that influence regional observations in recent field campaigns are being investigated through receptor models like positive matrix factorization (PMF) and transport receptor models like the potential source contribution function (PSCF). Expanded multilinear models are being considered to improve solutions including incorporation of additional information, e.g., wind data or atmospheric parameters.

Aerosol routes for the synthesis and pulmonary delivery of nanoparticle drugs:

Studies are being carried out in two broad areas.

a)The rational design of aerosol delivery systems with nano-sized drug encapsulating agents addressing issues of biocompatibility with the lung surfactant, drug encapsulation efficiency, lung deposition efficiency and reduced shear damage during aerosolisation.

b)Aerosol reactors for the synthesis of nanoparticle drugs with potential advantages like better control over the size distribution, reduced post-processing steps and continuous mode of operation.

Selected publications:

- S.G. Bhanuprasad, C. Venkataraman, M. Bhushan (2008) Source identification using positive matrix factorization and trajectory modelling: A new look at the INDOEX ship-observations, Atmospheric Environment, in press.
- Verma, S., C. Venkataraman, O. Boucher, and S. Ramachandran (2007), Source evaluation of aerosols measured during the Indian Ocean Experiment using combined chemical transport and back trajectory modeling, Journal of Geophysical Research, 112, D11210, doi:10.1029/2006JD007698.

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Systems and Synthetic Biology; Analysis of Genetic regulatory networks and signaling pathways; Metabolic Engineering; Bioreaction Kinetics; Microbial interaction in mixed cultures

Genetic regulatory networks: Development of dynamic/steady state models for genetic regulatory network. Quantification of microarray data using steady state models to infer the mechanistic details of genetic regulation. Analysis and design of synthetic genetic networks using open loop components. We have developed a strategy to analyze genetic networks using control analysis.

Signaling pathways: Application of steady state and dynamics modeling approach to signaling pathways in S. cerevisiae. Integration of multiple signaling cascades to gain insights into the regulation of filamentous growth response and osmoadaptation. Modeling cell cycle dynamics. We have extended the approach to study insulin signaling pathway in mammalian system.

Metabolic Engineering: Elementary mode analysis to quantify metabolic fluxes towards phenotypic characterization. Use of elementary modes to determine the phenotypic heterogeneity in cell cultures. Currently, we are extending the approach to obtain the kinetics of metabolism and growth.

- **Mixed culture systems:** B. subtilis resort to cannibalism under nutritional stress. However, our research group for the first time has demonstrated that B. subtilis prefers predation over
- cannibalism in mixed cultures. This has profound impact in discovering new antibiotics that may be microorganism specific. We have also quantified the interaction between species through kinetic models.

- **Selected Publications:**
- Quantitative analysis of GAL genetic switch of Saccharomyces cerevisiae reveals that nucleocytoplasmic
- shuttling of Gal80p results in a highly sensitive response to galactose, Malkhey Verma, Paike Jayadeva Bhat, and K. V. Venkatesh, The Journal of Biological chemistry, 278 (49), 48764-48769, 2003

Analysis of optimal phenotypic space using elementary modes as applied to Corynebacterium glutamicum, Kalyan Gayen and K.V. Venkatesh, BMC Bioinformatics, 7,445, 2006.

Integration of global signaling pathways, cAMP-PKA, MAPK and TOR in the regulation of FLO11, P. K. Vinod, Neelanjan Sengupta, P. J. Bhat and K. V. Venkatesh, PLoS ONE, 3(2): e1663, 2008

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Drying of thin film coatings, fluid mechanics of coating processes

Drying of polymer solvent coatings: Drying behaviour of single and multi-layer solution coatings made by dissolving a polymer in a solvent or multiple solvents is investigated. Several theories have been proposed for diffusion in polymer solvent systems involving a polymer and multiple solvents. These theories are being tested rigorously by comparing their predictions with experimental results. Operating conditions of dryers are optimized to produce defect-free coatings that meet residual solvent specifications.

Flow through porous media as applied to oil recovery: In secondary recovery process, water pumped through injection wells displaces oil to production wells from where it is recovered. Horizontal wells gained popularity over vertical wells because of their enhanced productivity and injectivity. The performance of these wells is measured and analyzed as a function of reservoir properties through experiments, modeling and simulation. Another area of study is flow in reservoirs with bottom water conditions. Yet another area is flow through fractured reservoirs.

Dehydration of foods: It is a common knowledge that dehydration of foods enhances their shelf life. Most of the earlier studies on drying of foods are empirical. Typical drying curves for foods are predicted from fundamentals of transport and drying conditions are optimized.

Selected Publications:

- Vinjamur, M. and Cairncross, R. A., A non-Fickian non-isothermal model for drying of polymer coatings, AIChE J, 48(11), 2444-2458, 2002.
- Nanji, H., Chaudhari, L., Mitra, S. K., Vinjamur, M. and Singh, R., Effect of scaling parameters on waterflood performance with horizontal and vertical wells, Energy and Fuels (accepted for publication, available online)
- Santosh, V., Mitra, S. K., Vinjamur, M. and Singh, R., Experimental and numerical investigation of waterflood profiles with different well configurations, Energy and Fuels, 21(6), 3353-3359, 2007.
- Nanji, H., Chaudhari, L., Mitra, S. K., Vinjamur, M. and Singh, R., Experimental investigation of use of horizontal wells in waterflooding, Journal of Petroleum Science and Engineering, 56(4), 303-310, 2007.

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Systems biology; Innate immune response; Noise distribution; Pattern formation

Innate immune response :
Dendritic cells (DCs) are sentinels of human innate immune system. They are emerging as an important target for new therapeutic strategies to combat infections and other diseases. DCs detect, capture, and process pathogens such as virus or bacteria. The processing of pathogens, orchestrated by a complex signaling network, regulates several genes. We use systems biology based approaches to understand the gene regulation mechanisms during various stages of DC response following infection.

Noise distribution and propagation in signaling pathways : Cell-to-cell variability plays an important role in cellular decision-making process. Cells take advantage of this variability, also called noise, to direct information processing via appropriate pathways in a signaling network. Noise transmits through the network. We study the effect of pathway properties on the distribution and propagation of noise in signaling pathways.

Pattern formation in packed-bed reactors: Spatiotemporal temperature patterns may form in packed-bed reactors during an exothermic catalytic reaction, pose severe safety issues and are detrimental to the reactor performance. Using mathematical modeling and bifurcation analysis, we investigate the mechanisms governing pattern formation and the conditions under which they may form.

Selected Publications:

- Viswanathan GA;Seto J;Patil S;Nudelman G;Sealfon SC. "Getting started in biological pathway construction and analysis". PLOS Computational Biology 2008;4:e16.
- Viswanathan GA;Nudelman G;Patil S;Sealfon SC. "BioPP: A tool for web-publication of biological pathways". BMC Bioinformatics 2007;8:168.
- Sundarram S;Viswanathan GA;Luss D. "Reactor diameter impact on hot zone dynamics in an adiabatic packed bed reactor", AIChE J. 2007;53:1578-1590.
- Viswanathan GA;Luss D. "Hot zones formation and dynamics in long adiabatic packed-bed reactors". Ind. Eng. Chem. Res., 2006;45:7057-7066.

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Computational structural biology, Experimental and theoretical analysis of Bioprocesses

Computational Structural Biology:
The objectives include the understanding of evolutionary relationship between proteins, gleaning information about active sites in proteins, discovery of novel secondary structures, fragment-based protein modeling and new drug design based on geometric concepts. We attempt to combine knowledge from three different fields; viz, biology, computational geometry and data-mining.

Physiologically Based Pharmacokinetic Modeling: Physiologically based pharmacokinetic models describe how foreign substances (e.g. drugs and toxins) are processed in the body by absorption, distribution, metabolism, and excretion. Our research consists of the following key sub-goals: (1) Molecular Level Models to predict physicochemical and biochemical characteristics of drug molecules; (2) Fluid Flow Models to account for variability due to blood perfusion in various sub-populations. (3) System Level Models and Integration: We plan to model whole-body physiological level phenomena and also account for the genetic variability in different subpopulation types. The molecular level and fluid dynamics level information will be integrated into the physiological level model using systems and feedback control theory.

Selected Publications:

- Bapat, P. M., Bhartiya, S., Venkatesh, K. V., Wangikar P.(2006), "A structured kinetic model to represent the utilization of multiple substrates in complex media during rifamycin B fermentation." Biotechnol. Bioeng., 93, 779-790.
- Tendulkar, A. V., Sohoni, M. A., Ogunnaike, B. and Wangikar, P. P. (2005), "A geometric invariant-based framework for the analysis of protein conformational space", Bioinformatics, 21, 3622-3628
- Tendulkar, A. V., Joshi, A A., Sohoni, M. A., Wangikar, P. P. (2004), "Clustering of protein structural fragments reveals modular building block approach of nature." J. Mol. Biol., in press.
- Tendulkar, A. V., Wangikar, P.P., Sohoni, M. A., Samant, V. V., Mone, C. Y. (2003) "Parameterization and Classification of Protein Universe via Geometric Techniques". J. Mol. Biol., 334, 157-172

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Post Doctoral Research (Laboratoire de Physique Statistique, Paris, 1995-1997)
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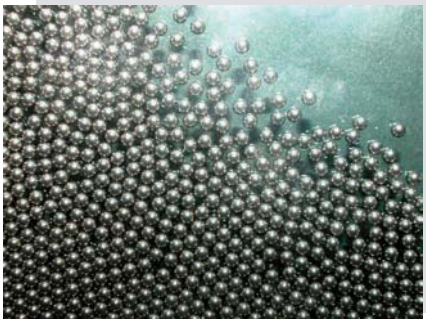
Research Interests:
Scattering techniques to study the structure of macromolecules and structure factor calculations using different models for the interaction potentials; Rheological studies on shear induced transitions in surfactant solutions; Self-diffusion measurement using FRAPP (fluorescence recovery after fringe-pattern photobleaching) on viscoelastic micellar solutions of monomeric and dimeric surfactants; Sol-gel transitions in biopolymers using absorbance and dynamic light scattering; Protein-protein and protein-surfactant interactions using static and dynamic light scattering, small angle x-ray scattering and suitable statistical mechanical models; 2D colloidal crystallization driven by AC field: Interpretation of the assembly and dissolution processes under different experimental conditions.

Selected Publications:

- "Salt Induced Liquid-Liquid Phase separation of Protein-Surfactant Complexes", Janaky Narayanan and Vinod W. Deotare, Phys. Rev. E 60, 4597 (1999).
- "Protein Interactions in Undersaturated and Supersaturated Solutions: A Study Using Light and X-ray Scattering", Janaky Narayanan and X. Y. Liu, Biophys. J. 84, 523 (2003).
- "Topology Evolution and Gelation Mechanism of Agarose Gel", Jun-Ying Xiong, Janaky Narayanan, Xiang-Yang Liu, Tan Kok Chong, Shing Bor Chen, and Tai-Shung Chung J. Phys. Chem. B 109, 5638 (2005).
- "Investigation on the Mechanism of Crystallization of Soluble Protein in the Presence of Nonionic Surfactant", Yanwei Jia, Janaky Narayanan, Xiang-Yang Liu, and Yu Liu, Biophys. J. 89, 4245 (2005).
- "Colloidal Phase Transition Driven by Alternating Electric Field", Yu Liu, Janaky Narayanan, and Xiang-Yang Liu, J. Chem. Phys. J. Chem. Phys. 124, 124906 (2006).



Film Production Equipment
Polymer Engineering Laboratory

- Isothermal titration calorimeter
- High performance liquid chromatography
- Atomic absorption spectrometer
- Zeta meter and particle size analyzer
- Thermal analyzer (DSC, DTA, & TGA)
- High temperature simultaneous thermal analyzer
- Cryo-Scanning electron microscope(Cryo-SEM)
- Energy dispersive xray attachment
- Image analyzer & optical microscopes
- Microscope hot stage
- Reaction injection moulding machine
- Universal testing machine
- Supercritical fluid extractor prototype plant
- Controlled stress-controlled rate rheometer
- Gas chromatographs
- UV - VIS spectrophotometer
- Gel permeation chromatograph
- Small angle xray spectrophotometer
- Single screw extruder
- Cast film and blown film assemblies
- High speed camera
- Fermenters
- Protein analysis system
- Incubators
- Laminar flow hoods
- Langmuir-Blodgett Trough
- Surface tensiometer
- Reactive distillation setups
- Laser particle size analyzer

Scanning Electron Microscope

Micro Lab

major recent projects (1999 - 2003)

- **Improved Granular Processing in Cement Manufacture**
  CSIR
- **Development of on-line fault detection & diagnosis (FDD) methodologies in integrated scale complex plants**
  BRNS
- **SAXS facility**
  DST
- **Adsorption of hydrocarbon gases on microporous material**
  MHRD
- **Elasticity and Photo-elasticity of thermoplastic Elastomeric Networks**
  DST
- **Photochemical oxidation of industrial organic pollutants in water using TiO2 catalyst in fluidized bed reactor**
  MHRD
- **Strengthening the teaching and research activities in the area of Colloid and Interfacial Engineering**
  MHRD
- **Development of versatile, portable software for Bioinformatics**
  CSIR
- **Development of Bio-Informatic Platform for Organisation, Modelling and Stimulation of Genetic Expression Data**
  MHRD
- **Rig Based Experiments: Modern Undergraduate Lab. in Chemical Engineering**
  MHRD
- **The feasibility analysis of potential reactive distillation systems**
  DST
- **Intracellular Reaction Rule (Flux) Analysis for Optimal Biosynthesis**
  MHRD
- **Development of Technology for Production of Electrical Grade Oriented PVDF Films**
  Bhabha Atomic Research Centre
- **Studies on the importance of wetting in detergency**
  Hindustan Lever
- **Study of the potential of ferrofluids in mass transfer intensification**
  Newreka Chemicals
- **Static and Dynamic aspects of microstructure formation when surfactant and surfactant / particulate mixtures contact water**
  Hindustan Lever
- **Improvement of Enzyme Productivities from Shear- sensitive Aerobic**
  DST
- **Application of Plant (Peroxidases & Lactases) for removal of recalcitrant organic Chemicals and dyes from Industrial Wastewater**
  DST
- **Wastewater recycling via vermiculture biofilters**
  AICTE
- **Studies in reaction for electrochemical methods for effluent treatment**
  AICTE
- **Prediction and characterization and equilibria and dynamics of polymer adsorption on solid surfaces**
  Hindustan Lever
- **Polymerization of aramid polymers under programmed shear flow conditions**
  Naval Research Board
- **Mixing and segregation of granular materials**
  DST

AICTE: All India Council for Technical Education
BRNS : Board for Research in Nuclear Sciences
CSIR : Council for Scientific and Industrial Research
DST : Department of Science and Technology
MHRD: Ministry of Human Resource Development

patents

Faculty member	Title
A K Suresh (aksuresh@che.iitb.ac.in)	An enzymatic hydrolysis process for the production of glucose syrups from tapioca starch. An enzymatic hydrolysis process for the production of liquefacts (maltodextrins) from tapioca starch.
K C Khilar (kartic@che.iitb.ac.in)	A low temperature process for the synthesis of rutile TiO_2 nanoparticles and TiO_2 particles coated with zinc oxide.
A Moharir (amoharir@che.iitb.ac.in)	PSA based medical oxygen technology.
S R Patwardhan (srp@che.iitb.ac.in)	Process for production of 95% carbozole from coal tar.
M Mukhopadhyay (mm@che.iitb.ac.in)	A process for sequential supercritical CO_2 extraction and fractionation of Neem oil enriched with Azadirachtin from Neem Kernels. A process for cyclic supercritical fluid CO_2 extraction of fragrances from Jasmine flowers.
G K Sureshkumar (gksuresh@che.iitb.ac.in)	A process for preparation of granulated non-living biomass of a fungus for sorption of toxic trace heavy metals and organic chemicals from effluents.
H S Shankar (hss@che.iitb.ac.in)	Process for waste water renovationProcess for treatment of organic solid waste.
J Bellare (jb@che.iitb.ac.in)	A method of making a supported fluid separation membrane of nanopore structure. A method of making a fluid separation material such as membrane of nanopore structure. Improvements related to Clinical thermometers. Automatic flow-through refractive index sensor. A single-chip dip-probe for refractive index measurement. A controlled environment vitrification system for electron microscopy of liquid. A process to manufacture highly stable and optically transparent aluminum hydroxide gel. A process to manufacture nostrandite of high yield from aluminum alkoxide. Preparation of crack-free, enhanced selectivity alumina membranes from chelated aluminum secondary butoxide. Pore size tailorability in alumina membranes using surfactant micelles as templates. Surfactant formulations with adjuvants for neonatal and adult respiratory distress syndromes.

technologies transferred

Faculty (Group)	Technology Transferred
M. Mukhopadhyay, S. Roy, S. Baser	Supercritical Fluid (Carbon Dioxide) Extraction Technology for Natural Products
H. S. Shankar	Vermiculture Technology for Solid and Liquid Waste management
K. V. Venkatesh N. G. Shah (CTARA)	Palletized Tea Storage Methodology employing Controlled Atmosphere
A. S. Moharir	Design Analysis and Simulation of Batch Distillation and Pressure Swing Adsorption Unit
J. Bellare	Design & Development of Vertically Integrated pilot plant for Optical Glass Fibers for Light Guide and Image Guide Applications (used in biomedical optics for endoscopy)
	Continuous Pressing Plant for Membrane Production for use in Microfiltration of Pharmaceutical Products and in Biomedical Devices
	Biodegradable LDPE Technology
	Integrated Jewellery Manufacturing Plant with Automatic Vacuum Recovery and CNC / Robotics Production

Supercritical Fluid Extraction Pilot Plant

Thermodynamics lab

The Department interacts closely with industry through collaborative research, projects and the other services it offers. It also provides services to other institutions like colleges and research organizations. A list of typical services is given below.

1. Analytical / Numerical Modelling & Simulation

2. Process Development

3. Specialized Experiments

4. Technology Evaluation

5. Special Materials Development

6. Fundamental Research

7. Material Characterization and Testing

8. Advanced & Practice-Oriented Continuing Education Programs

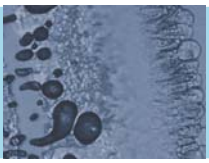
9. Professional Development and Training of Teachers from other Institutions

Simultaneous Thermal Analysis System

Organic Process Laboratory

faculty awards

NAME OF THE AWARD	RECEPIENT	YEAR
S.S. BHATNAGAR [CSIR]	D.V. KHAKHAR	1997
HERDILLIA [IICHE]	V.A. JUVEKAR	1997
	D.V. KHAKHAR	1999
	A.K. SURESH	2000
ICI [IICHE]	JAYESH BELLARE	1997
HINDUSTAN DORR - OLIVER [IICHE]	H.S. SHANKAR	1997
	K.V. VENKATESH	2005
NOCIL [IICHE]	M. MUKHOPADHYAY	1997
	SANDIP ROY	1997
	S. A. BASER	1997
AMAR DYE - CHEM [IICHE]	D.V. KHAKHAR	1993
	ANURAG MEHRA	1994
	U.V. SHENOY	1995
	K.V. VENKATESH	1998
	S.M. MAHAJANI	2002
P. K. PATWARDHAN AWARD	M. MUKHOPADHYAY	2001
	SANDIP ROY	2001
	S. A. BASER	2001
FELLOW, INDIAN NATIONAL ACADEMY OF ENGINEERING	A. MISRA	1996
	D.V. KHAKHAR	2000
	K.C. KHILAR	2003
FELLOW, INDIAN ACADEMY OF SCIENCES	D.V. KHAKHAR	1996
FELLOW, INDIAN NATIONAL SCIENCE ACADEMY	D.V. KHAKHAR	2002
FELLOW, NATIONAL ACADEMY OF SCIENCES	A. MISRA	2001
FELLOW, MAHARASHTRA ACADEMY SCIENCES	A. MISRA	2001
ASSOCIATE INDIAN ACADEMY OF SCIENCES	ANURAG MEHRA	---
YOUNG SCIENTIST, INDIAN NATIONAL SCIENCE ACADEMY	ANURAG MEHRA	1989
	K.V. VENKATESH	1999
YOUNG ENGINEER, INDIAN NATIONAL ACADEMY OF ENGINEERING	K.V. VENKATESH	1998
	S.A. BASER	2000
SWARNAJAYANTI FELLOWSHIP [DST]	D.V. KHAKHAR	1998
	K.V. VENKATESH	2004
EUROPEAN COMMISSION FELLOWSHIP [EC AND DST]	ANURAG MEHRA	1995
BOYSCAST FELLOWSHIP, DST	P. WANGIKAR	2004



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