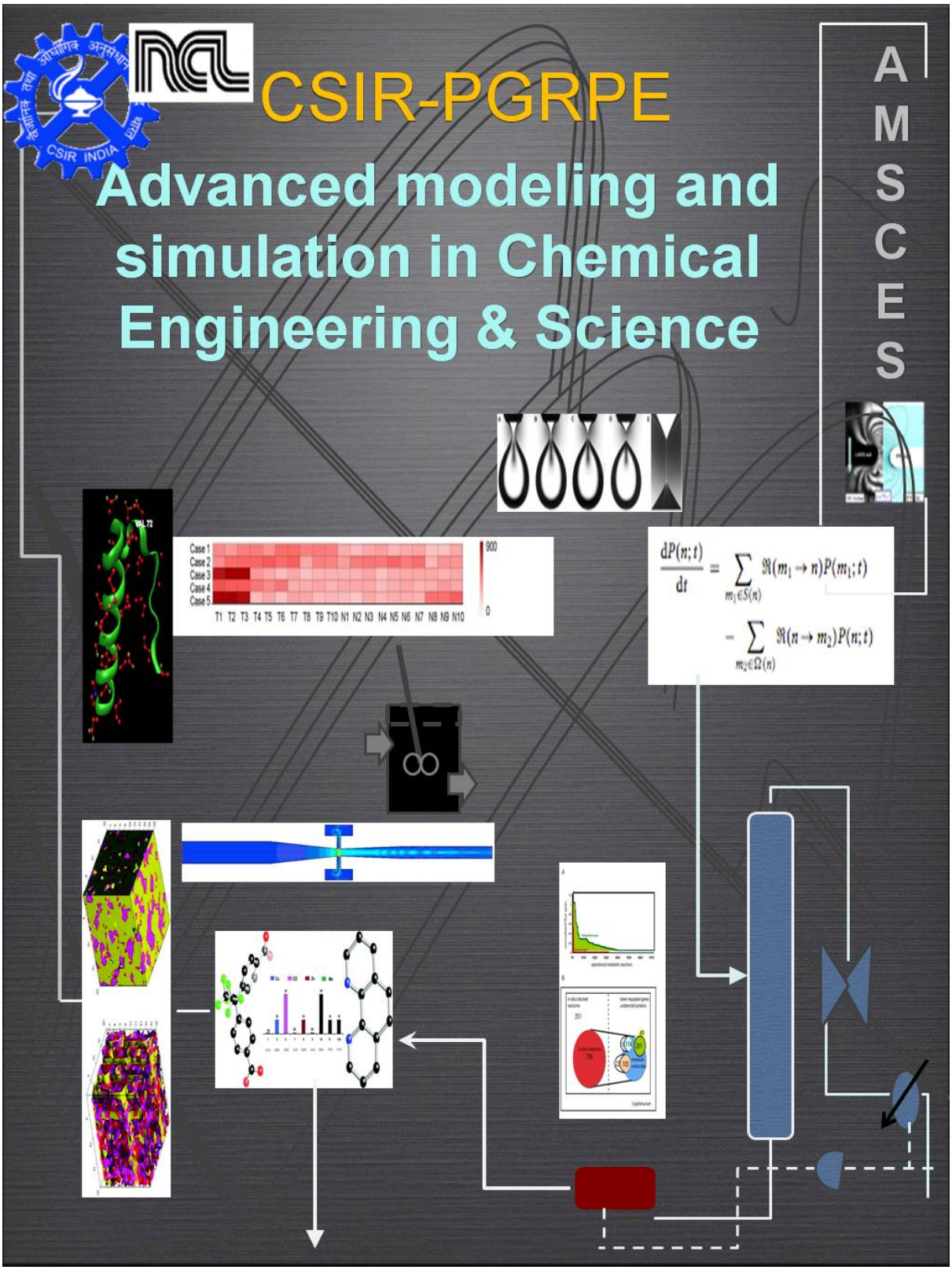


BROCHURE FOR CLASS OF 2010-12

Table of Contents

Summary

Objective

To impart training in advanced modeling and simulation techniques and application of these techniques to problems in chemical engineering and science.

Eligibility

4-year Bachelors degree in a discipline associated with Chemical Engineering/Technology. Examples are Chemical Engineering, Chemical Technology, Polymer Engineering, Biochemical Engineering, Materials Science and Engineering, Petroleum and Petrochemical Engineering. Other eligibility criteria as per CSIR guidelines. Currently industry-sponsored candidates or foreign nationals are not eligible.

Duration

Two years

Mode of operation

Currently for full-time students only. Part-time modes may be introduced later, possibly for industry-sponsored students.

Number of seats

Maximum of 10

Finances

Fees as per CSIR guidelines. Payment of fees for selected students only (not application fees if any) to be paid through a DD to “Director, NCL” payable at Pune. Details will be posted at NCL’s PGRPE website. Financial assistance will be provided as per CSIR guidelines.

Application procedure and selection criteria

As per CSIR Post Graduate Research Program in Engineering application procedure: details at http://www.csir.res.in/csirpgrp/pgrpe.htm

Program Description

The academic program comprises of 12 subject courses including wet-lab and symposium, and one project, for a total of 70 credits. One credit approximately corresponds to 15 faculty-student contact hours. In addition, students are expected to spend approximately twice that time in self-study, assignments, and course projects. Evaluations are biased towards a continuous mode, with at least half the total marks assigned for performance in classroom tests, and homework assignments. There will be a mid-semester and end-semester exam at defined times, which may also be in the open-book or take-home format. Emphasis will be on understanding and implementation rather than accumulation of facts. One credit courses will be offered on a Pass/Fail basis during the inter-semester periods

Semester I

The first semester comprises of five courses that form the core courses in the program.

Summary

S. No.	Subject	Code	Hours/week	Duration	Credits
1	Mathematical fundamentals	MSC01	3	20 weeks	4
2	Numerical methods and programming	MSC02	3	20 weeks	4
3	Transport phenomena	MSC03	3	20 weeks	4
4	Thermodynamics and statistical mechanics	MSC04	3	20 weeks	4
5	Reaction and reactor engineering	MSC05	3	20 weeks	4
Total			*Average 15hours/week*		*20*

Semester II

The second semester comprises of five specialized courses that introduce the student to specific areas where modeling and simulation is employed, and domain-specific principles and techniques. Additional courses may be offered, in which case students will have the option of choosing specialized courses to fulfill their course credit requirements. In addition, the student is supposed start preliminary work for their research project.

Summary

S. No.	Subject	Code	Hours/week	Duration	Credits
1	Multiscale simulations in materials	MSE01	3	20 weeks	4
2	Industrial flow modeling	MSE02	3	20 weeks	4
3	Data driven modeling	MSE03	3	10 weeks	2
4	Non-linear system dynamics	MSE04	3	10 weeks	2
5	Modeling of biological systems	MSE05	3	20 weeks	4
Total			*Average 12 hours/week*		*16*

Semesters III and IV

The third and fourth semesters will involve research with a scientist-mentor. Co-advised projects, or projects with both experimental and modeling/simulation components may be offered. The student is expected to work in the scientist's lab and interact with him/her daily. There will be an evaluation every 12 weeks, with detailed reports on the progress of the project and plans for the next 12 weeks to be presented to either the instructor or a committee, who will evaluate the candidate based on the report and an oral presentation.

Semester III

S. No.	Subject	Code	Duration	Credits
1	Project evaluation I	MSP01	12 weeks	4
2	Mid-project evaluation	MSP02	12 weeks	8
	Total		*24 weeks, 12 credits*	

Semester IV

S. No.	Subject	Code	Duration	Credits
1	Project evaluation III	MSP03	12 weeks	4
2	Final Project evaluation	MSP04	12 weeks	16
	Total		*24 weeks, 20 credits*	

Course details

MSC01: Mathematical fundamentals **4 credits**

Course Objective

To review mathematical fundamentals, teach common mathematics prerequisites of other courses, and to impart perspective on modeling and simulation.

Modules

- Analysis basics
- Probability basics
- Linear Algebra
- Ordinary and partial differential equations
- Statistical models and methods
- Optimisation

MSC02: Numerical Methods and Programming **4 credits**

Course Objective

To understand the algorithms involved in the numerical methods used for computer simulation, have the ability to choose an appropriate algorithm and be aware of the advantages and pitfalls expected in a particular algorithm. Computer implementation of algorithms and use of Matlab or other subroutines.

Modules

- Introduction to Programming, linux
- Introduction to Matlab/Scilab/Octave
- Matrix operations
- Function approximations
- Solutions of system of nonlinear equations
- Numerical methods for ODEs
- Finite-difference/volume methods for PDE
- Finite element methods
- Optimization approaches

MSC03: Transport phenomena **4 credits**

Course Objective

To develop a good physical understanding of the processes of momentum, heat and mass transfer at the continuum level; to develop the mathematical tools to quantitatively solve problems in transport phenomena

Modules

- Linear algebra and calculus relevant to transport phenomena
- Conservation equations
- Examples in transport phenomena

MSC04: Thermodynamics and Statistical Mechanics **4 credits**

Course Objective

To develop the understanding of thermodynamics principles as applicable to chemical systems.

Modules

- Classical Thermodynamics, ideal gases
- Solution thermodynamics
- Equilibrium thermodynamics
- Non-equilibrium thermodynamics
- Ensemble methods

MSC05: Reaction and Reactor Engineering **4 credits**

Course Objective

To develop the understanding of the reactions from molecular scale to the reactor scale, and to equip the student to model different reactor configurations and non-idealities in reactor systems.

Modules

- Chemical kinetics
- Homogeneous reactor analysis and design
- Heterogeneous reactor analysis and design
- Special reactors

MSE01: Multiscale simulations in materials **4 credits**

Course Objective

To be familiar with simulations at the molecular and sub-molecular scale, including quantum chemistry based and classical mechanics based methods.

Modules

- Introduction to molecular modeling
- Quantum-chemistry driven modeling
- Classical mechanics based modeling
- Example problems at multiple scales

MSE02: Industrial flow modeling **4 credits**

Course Objective

To teach students the basic equations of fluid dynamics and computational methods to solve these equations as applied to flows in industrial processes. At the conclusion of the course students will be able to analyze complex flow situations, develop a simple model for complex flow and solve it numerically, and simulate the actual complex flow using available CFD software.

Modules

- Introduction to CFD
- Solution techniques for solving CFD equations
- Introduction to CFD Software
- Turbulence modeling
- Multiphase flows

MSE03: Data driven modeling **2 credits**

Course Objective

The course will emphasize the conceptual understanding of methods along with their implementation in real world scenarios. At the end of the course, the student is expected to be able to be able to identify and implement appropriate conventional, machine learning or AI based methods for linear/non linear data fitting, data reduction, and classification.

Modules

- Statistics basics
- Supervised learning
- Unsupervised learning
- Artificial intelligence based methods
- Model validation
- Practical applications in data reduction, feature selection, classification.

MSE04: Non-linear dynamics **2 credits**

Course Objective

Introduce methodologies for analyzing complex nonlinear behavior with examples from reaction engineering, chemical, and physical systems. Students will learn (1) how nonlinear systems differ from linear systems regarding their dynamical properties; (2) how to analyze the stability of complex systems ; (3) how sensitivity of system dynamics is related to predictability and control; (4) to explore dynamical systems analytically and with computer simulations

Modules

- Introduction to the dynamics of nonlinear systems
- Preliminary analysis of time-series data:
- Toy “Nonlinear models” and the role of parameters
- Stability of solutions to ODEs
- Properties of chaos:
- Self organizing properties of nonlinear systems
- Phase space analysis

MSE05: Modeling of biological systems **4 credits**

Course Objective

Provide a brief background of biological systems for model development. Bioreactor design and analysis. Metabolic network modeling using constraint based approaches and signaling pathway modeling using deterministic and stochastic modeling techniques.

Modules

- Biological fundamentals
- Bioreactor models
- Metabolic pathways
- Signaling pathways
- Pharmacokinetics and pharmacodynamics

MSP01-04: Project **32 credits**

Course Objective

Provide hands-on experience in collection and critical analysis of available literature in a given area and formulation of a research proposal. Planning and execution of the proposal in close association with a scientist-mentor. A faculty advisor will monitor progress on a regular basis, in addition to the formal evaluations every 12 weeks.

MSL01-03: Wet-Lab **01 credit**

Course Objective

Provide hands-on experience in collection of data and analysis of experimental results in three areas: Biology, Complex fluids, and Industrial Flow.

MSS01: Symposium participation **01 credit**

Course Objective

Provide exposure to current topics through scientific talks and poster session, and an opportunity to showcase research ability and results to potential employers. Students are expected to present posters and interact with participants from industry and academia.

Faculty Profiles

Name/Contact details	Education and Experience	Research Interests
Dr. Amol A. Kulkarni Scientist NCL Phone: 020-25902153 E-mail: aa.kulkarni@ncl.res.in 	• IUSSTF Research fellow, MIT, Cambridge, USA • Postdoctoral fellow, MPI for Dynamics of Complex Systems, Magdeburg, Germany • Ph.D., (Chemical Engineering), M. Chem. Eng., B. Chem. Engg.; Inst. of Chem. Technology (ICT, formerly UDCT).	• Microreaction technology: micro-fluidics, design of miniaturized devices, modelling and experimentation. • Continuous flow synthesis of API, nanoparticles and azo colorants • Experimental and computational fluid dynamics • Nonlinear dynamics • Development of data analysis techniques for nonlinear and non-stationary data
Dr. Anu Raghunathan Scientist, NCL Phone: 020-25903067 Email: anu.raghunathan @ ncl.res.in 	• Faculty (Research), Mount Sinai (Medicine), NY • Post doctoral Fellow, Bioengineering, University of California San Diego • Post Doctoral Fellow, Microbiology and Cell Science, Univ of Florida • Ph.D., Chemical Engineering, IIT Bombay • M.S., Analytical and Medicinal Chemistry, SNDT, Mumbai	• Metabolic network reconstruction and constraints based analysis of biological systems • Microbial strain design for use of renewable resources, systems biology and molecular adaptation to produce and improve yields. • Drug Target Discovery: Systemic approaches (computational and experimental) to study metabolism in pathogenesis to discover novel drug targets.
Dr Ashish Lele Scientist, NCL Phone:020-25902199 Email: ak.lele@ncl.res.in 	• Research Associate, University of Cambridge • Ph.D., Chemical Engineering, University of Delaware, USA • B.Chem.Eng., University of Mumbai, Department of Chemical Technology (UDCT)	• Rheology of complex fluids such as polymer melts, associating polymer solutions and soft solids. • Developing coarse-grained models for polymer dynamics and using them to quantify the processing behavior of melts in complex flows by a combination of CFD simulations and experimental validation. • Structure-property relations in physical gels
Dr. Ashish Orpe Scientist, NCL Tel: 020-25902749 Email: av.orpe@ncl.res.in 	• Postdoctoral Research Associate, (2004 – 2007), Department of Physics, Clark University, MA, USA • Ph.D., Chemical Engineering, (2004), IIT Bombay, Mumbai, India • M.Tech., Chemical Engineering, (1998), IIT Bombay, Mumbai, India • B. E., Petro-Chemical Engineering, Univ. of Pune,	• Dynamics and structure of sheared, dense granular flows. Mixing and segregation behaviour in granular media • Exploring three dimensional dynamics in large scale multi-phase systems • Micro-rheology (dynamics and structure) of sheared dense colloidal dispersions using fast scanning confocal microscopy

Name/Contact details	Education and Experience	Research Interests
Dr B. D. Kulkarni Scientist, NCL Phone:020-25902150 Email: bd.kulkarni@ncl.res.in 	• PhD, Chemical Engineering, University of Pune • M. Tech, Chemical Engineering, LIT, Nagpur • B Tech Chemical Engineering, LIT Nagpur	• Chemical reaction engineering • Mathematical modeling • Optimisation and control • Process design • Fluidization • Microemulsions/ micelles
Dr Chetan Gadgil Scientist, NCL Phone: 020-25902163 Email: cj.gadgil@ncl.res.in 	• Investigator, GlaxoSmithKline, USA • Postdoctoral research associate, School of Mathematics, U. Minnesota • Ph.D., Chemical Eng, Univ. of Minnesota, USA • M Tech, Chemical Engineering, IIT Bombay • B. Chem. Eng. ICT (formerly UDCT), Mumbai.	• Mechanistic models of biological systems: regulatory networks, other cellular processes • Modeling/Simulation of patterning in biology • Stochastic models for (bio) chemical reactions • Modeling drug delivery and distribution kinetics
Dr. K. Guruswamy Scientist, NCL Phone: 020-25902182 Email: g.kumaraswamy@ ncl.res.in 	• Postdoctoral fellow, Max Planck Institute for Colloids and Interfaces, Germany • Ph.D., Chemical Engineering, California Institute of Technology, USA. • M.S., Chemical Engineering, California Institute of Technology. • B.Tech., Chemical Engineering, Indian Institute of Technology, Bombay.	• Synthesis and assembly in anisotropic liquid crystal matrices • Plate-like anisotropic nanoparticles – self-assembly & nanocomposites • Rheology and structure of two-phase (crystallizing) polymer melts
Dr Kumar Vanka Scientist, NCL Phone: 020-25902083 Email: k.vanka@ncl.res.in 	• Postdoctoral fellow, (CEBC), Kansas University • Ph.D., Chemistry, University of Calgary, Canada. • M.Sc., Chemistry, University of Calgary. • BSc. Chemistry, Indian Institute of Technology, Khargapur.	• Determining catalytic routes to hydrogen storage • Finding better catalysts for asymmetric hydroformylation • Stochastic methods to study changes in reactant-product concentrations • Determining the principles behind polymer formation using Ziegler-Natta heterogeneous catalysts

Name/Contact details	Education and Experience	Research Interests
Dr Mugdha Gadgil Scientist, NCL Phone:020-25902433 Email: mc.gadgil@ncl.res.in 	• Scientist, Invitrogen Corporation, MD, USA • Postdoctoral research associate, University of Minnesota, MN, USA • Ph.D., Chemical Eng, University of Minnesota, MN, USA, 2004. • B. Chem. Eng. ICT (formerly UDCT), Mumbai, 1999.	• Bioinformatics: developing methods for analysis of DNA microarray data • Bioprocess engineering for cell culture processes
Dr Neelanjana Sengupta Scientist, NCL Phone: 91-20-25902087 Email: n.sengupta@ncl.res.in 	• PhD, Physical Chemistry, Univ. of California, Irvine, 2008 • M.S, Chemical & Materials Physics, Univ. of California, Irvine, 2007 • M.Sc, Physics, Univ. of Burdwan, 2000 • B.Sc, Physics, Univ. of Burdwan, 1998	• Understanding amyloid formation and protein aggregation diseases • Protein translocation through membranes • Solvent dynamical coupling in biomolecules • Transport and signaling phenomena in biomolecular confinement
Dr. Pankaj Doshi Scientist, NCL Tel: 91 20 25903074 Email: p.doshi@ncl.res.in 	• Principal Scientist, Pfizer Inc, USA • Investigator, GlaxoSmithKline, USA • Postdoctoral researcher, MIT, Cambridge, MA, USA • PhD, Chemical Engineering Purdue University • M.Tech., Chemical Engineering IIT Bombay • B.Tech., Chemical Engineering IIT Bombay	• Numerical Simulation of free surface flow of Newtonian and non-Newtonian fluids: Finite element method, Steady and Time dependent simulation, Parallel Computing; Interfacial flows; Study of inkjet printing, liquid drops and jets • Computational models, design and optimization of Dry Powder Inhaler, design of novel drug formulations • Mathematical models for design, control and optimization of pharmaceutical unit operations
Dr. V. Ravi Kumar Scientist, NCL Tel: 91 20 25902161 Email: v.ravikumar@ncl.res.in 	• Postdoctoral Research Associate, (1984 -1986), Department of Chemical Engineering, Texas A&M University, TX, USA • Ph.D., Chemical Engg. Division, National Chemical Laboratory & University of Pune, India • M.Sc., Chemistry Dept., Bangalore University , (1978)	• Nonlinear dynamics, chaos and turbulence • Chemical reaction engineering • Analysis of complex systems and networks • Parameter estimation, optimization and control • Noise reduction in nonstationary data by multiresolution techniques • Studying data classification, pattern formation and feature extraction from space-time data obtained from experimental systems

Name/Contact details	Education and Experience	Research Interests
Dr. Sanjeev Tambe Scientist, NCL Tel: 91 20 25902156 Email: s 	• Visiting Scientist, Department of Chemical Engineering, University of Louisville, KY, USA. • Research Associate at Department of Geology, University of Louisville, Louisville, KY, USA. • Ph.D, (Physical Chemistry) NCL & Univ. of Bombay • M. Sc. (Analytical Chemistry) Department of Chemistry, University of Bombay	• Design, development and application of Artificial Intelligence and machine learning formalisms to chemical and biological systems. • Modeling and optimization of reactions/reactors; control and analysis of nonlinear systems • Chemical reactor/reaction modeling via phenomenological, stochastic, cellular automata, and Monte Carlo approaches • Applications of fractal theory and multi-variate statistics.
Dr. Sourav Pal, Scientist, NCL Phone: 9120 2590 2001 Email: s. pal@ncl.res.in 	• Post doctoral research associate at University of Florida 1986-87 • Alexander von Humboldt Fellow, University of Heidelberg, Germany 1987-88 and several short periods subsequently • Ph D, IACS, Kolkata, 1983 • M Sc (5 years' Integrated) in Chemistry, IIT, Kanpur, 1977	• Electronic Structure theory for properties on spectra • Development of linear response formalism for effective Hamiltonian based theories. • Conceptual DFT for description of reactivity in molecules • Computational material science for catalytic properties of zeolites • Theoretical study of hydrogen storage properties of metal hydrides/ MOFs
Dr Sudip Roy Scientist, NCL Phone: 91-20-25902735 Email: s.roy@ncl.res.in 	• Postdoctoral Fellow; Technical University Darmstadt, Germany • Ph.D., Chemistry, Saarland University, Germany • M.Sc., Visva Bharati Central University, West Bengal • M.Sc, Physics, Univ. of Burdwan, 2000 • BSc. Visva Bharati Central University, West Bengal	• Prediction of macroscopic properties from molecular and mesoscopic scale simulations • Multiscale method development • Force field development and optimization for new systems for molecular dynamics simulations • Coarse graining of polymers and bio-molecules to simulate long time and larger length scale phenomena
Dr Vivek V Ranade Scientist, NCL Phone:91-20-25902170 Email: vv.ranade@ncl.res.in 	• Research Associate, ETH Zurich, 1988-90 • Ph.D., Chemical Engineering, University of Mumbai, Department of Chemical Technology (UDCT), 1988. • B. Chem. Eng., University of Mumbai, Department of Chemical Technology (UDCT), 1984	• Multiphase reactor engineering. • Developing multi-scale models to simulate large industrial flow processes/ Industrial flow modeling. • Developing methodology for bridging the gap between capabilities of state of the art mathematical models and industry requirements • Turbulent, multiphase flows/ phase change

NCL Research and Facilities

About NCL

- NCL, India is a research, development and consulting organization with a focus on chemistry and chemical engineering. It has a successful record of research partnership with industry.
- NCL belongs to the family of Council of Scientific and Industrial Research (CSIR).
- NCL's human resources comprise of over 1000 people of whom 200 are scientists with a PhD in science or engineering and over 300 students pursuing research leading to PhD degree.
- Over 400+ research papers in international journals.
- Over 70+ Indian and foreign patents granted to NCL

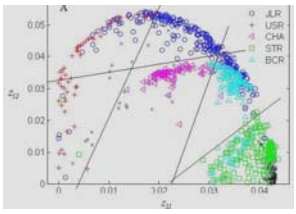
More information can be obtained from the intranet (newhome.ncl.res.in), academic site (ncl.res.in), or the business site (ncl-india.org).
Throughout the year, various conferences, invited talks, seminars, and other meetings are held at NCL, and are notified by email or postings at the NCL website. You are encouraged to broaden your horizons by attending talks in areas that may not seem to be directly relevant to your PhD research. This unique opportunity to attend talks by world-class researchers and technologists is one of the many advantages of being part of the NCL community. In addition, proximity and close interactions with the Indian Institute of Science Education and Research (IISER), Pune, and the NCL Venture Center give applied researchers the opportunity to carry out projects in basic sciences as well as get assistance with exploring the commercial implications of their research results.

Research in Modeling and Simulation @NCL

Current research activities at NCL include modeling and simulation at length scales ranging from the sub-atomic to chemical-plant scales. Several projects include a combined theoretical, computational and experimental investigation of a particular phenomenon. A glimpse of some of these activities is presented in the following sections, broadly divided into research in analysis of reactions, simulations at the single molecule and smaller scales, and flow simulations.

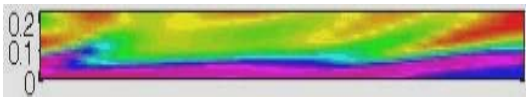
Reactor and reaction modeling

There are active research programs at NCL on both mechanistic and data-driven reactor modeling. Recently, NCL has established a Centre of Excellence on Microreaction Technology. Models for micro-reactors as well as conventional reactors such as bubble column reactors, trickle-bed reactors, gas-liquid stirred tanks, and polymer processing equipment have been developed. Models for fundamental processes such as drop formation and granular flows have been developed. Data-driven methods have been developed for flow regime identification, pattern detection and fault detection from chemical reactor and plant data. At the reaction scale, chemical and biochemical reaction networks are investigated using deterministic and stochastic methods. Data-analysis techniques have been used to analyze large-scale data from chemical and biological systems. Facilities for experimental studies at several scales are available and used in conjunction with modeling and simulation studies.



Ongoing research includes the elucidation of pattern formation, recognition and feature extraction in reacting systems using multiscale resolution techniques. The results also assess the predictability in the space-time behavior of complex systems and develop optimization, control and classification algorithms for high dimensional systems. The algorithms have especially found important applications in effective noise reduction of data

prior to mathematical modeling of even highly nonlinear processes. Nonlinear dynamics approaches are used to identify common principles responsible for order/disorder and pattern formation that arise in reaction engineering systems (CSTR; multiphase reactors; fixed bed; fluidized bed; mixing in channel flow, jet reactors, etc.). Consequently, these studies have helped to analyze experimentally monitored data obtained from these systems using sophisticated instruments like LDA, PIV HFA for its chaotic and turbulent properties.

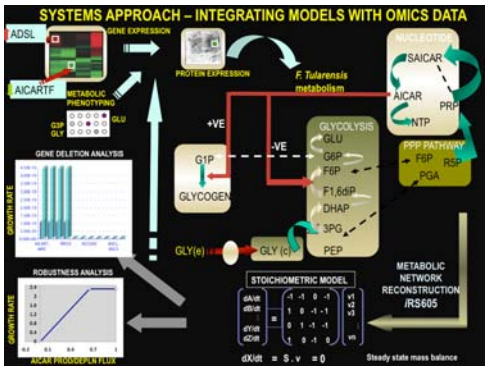


Artificial intelligence formalisms have been employed for steady-state and dynamic process modeling, nonlinear model-based control, process identification, process fault detection/diagnosis, soft-sensor development and process optimization from historical process data and in the absence of a detailed knowledge of the physico-chemical phenomena underlying the process. AI-based strategies for chemical processes have been developed.

Another research area involves kinetic modeling of reactions such as autoxidation of hydrocarbons, runaway decomposition reactions, reactive dissolution of polydisperse material. Methods for prediction of thermochemical properties are applied to estimation of properties of organic free radicals. For autoxidations the approach has been validated against observed behavior in both lab scale batch reactors and large scale continuous air-sparged reactors. The kinetic modeling of several complex multi-step (often free radicals-based) runaway decomposition reactions using adiabatic calorimeter data on the temperature-time or pressure-time profiles has opened up possibilities for design and scale up of reactors and provides tools for the discrimination of mechanisms in liquid phase oxidation (LPO) processes. Estimating the thermochemical properties of a large number of organic free radicals has been made possible using a database of group-additivity values. The methodology is useful in estimating properties of a wide range of radicals for mechanistic studies of LPO reactions and related decompositions.

In addition to chemical systems, modeling and simulation techniques are also applied for the analysis of complex biochemical systems. Autocatalytic biological systems are studied at various length and time scales; and specific systems such as autocatalytic production of the transcription factor TBP are investigated in collaboration with experimental biologists. In systems such as binding of a few protein molecules to one of two DNA sites in a cell, with a small number of molecules of each reactant, stochastic models are used. Theoretical and computational stochastic approaches are used for investigating systems with multiple steady states.

Research in the area of Systems Biology involves the integration of high throughput experimental data with genome-scale organism models to generate novel hypothesis and drive biological discovery. Enumeration of various cellular components and a description of their interactions allow formulation of a mathematical description of the totality of such interactions, identify constraints that the resulting network operates under, and apply optimality principles to compute likely physiological functions in a given environment. These capabilities provide a consistent framework on which a mechanistic basis for the microbial metabolic genotype– phenotype relationship can be established. Current research includes reconstruction of metabolic and signaling biochemical

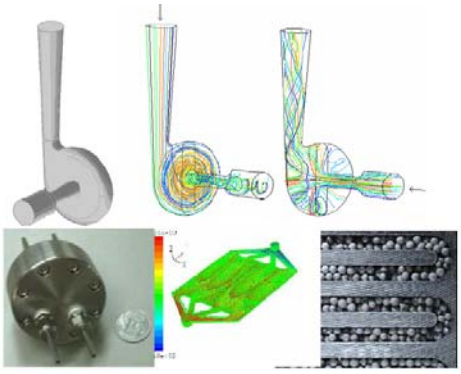


reaction networks in microbial and organelle systems, and constraints based modeling for computing cell function. These are applied to understand problems ranging from metabolic engineering to infectious disease and related drug/drug-target discovery. In addition, genome-scale metabolic models are used to predict rational strain design options that allow overproduction of desirable metabolic by-products. Constraints-based models of both the pathogen and the host allow the in silico study of host-pathogen interactions. Metabolic implication in infection and pathogenesis allows us to define a basis for new drug or drug target discovery.

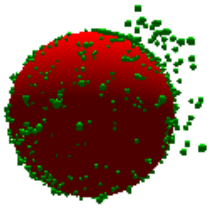
DNA microarray assays are used for the identification of differences in gene expression between two or more classes of samples, e.g., between disease and normal tissue. High throughput biological assays like DNA microarrays lead to the generation of large scale datasets whose analysis uses methods from statistics and machine learning. Research in this area aims at the development of new methods or analysis and identification of appropriate existing methods for specific experimental conditions. For example, a new statistical method has been developed for identification of differentially expressed genes between two groups especially for application in datasets with high 'within group' variability.

Flow modeling

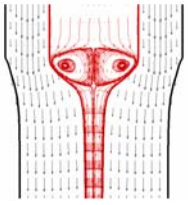
Current research in flow modeling aims at understanding the transport phenomena in multiphase reactors such as boiling reactors, trickle-bed reactors and gas-liquid stirred tanks and developing design and scale-up guidelines. Connecting the heat transfer at various levels/scales with the performance of the reactor is being studied by multiscale modeling. Developing new devices and continuous flow processes for microreactors is another thrust area. Microreactor processes are beign developed for synthesis of active pharmaceutical ingradients, azo dyes, perfumery esters and nanoparticles. Phenomenological models (for heat transfer and reaction engineering) or computational flow modeling of the miniaturized devices or fluidic devices like a vortex diode, passive micro mixers, etc. are developed to understand these processes.



In the area of powder flows, theoretical and experimental studies are underway to understand the physics of granular materials. Other than traditional materials processing applications, this research can be used to design drug delivery devices such as dry powder inhalers. A particle based technique, discrete element method, is being used to model the collective behavior of large number of fine particles. This computational method presents a convenient method to obtain insight into both microscopic and bulk behavior of particle systems. The ultimate goal of this research work is to develop a model for inhalers which takes into accounts physical and chemical properties of blend.

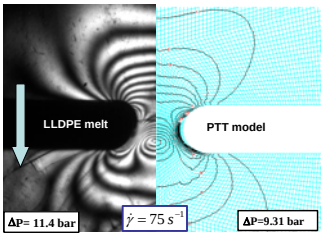


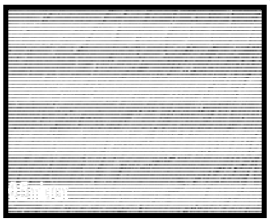
Computational approaches are extensively used for the design of fluidic devices. Various devices such as miniaturized fluidic devices like a vortex diode, passive micro mixers, etc are being studied through computational approaches. In recent years there has been considerable progress in inkjet printing of polymeric fluids for diverse applications such as bio-assays and multicolor polymer light-emitting diode displays. The printing of polymer involves formation of a drop and its subsequent impact and deposition on a substrate. Ongoing research aims to develop new

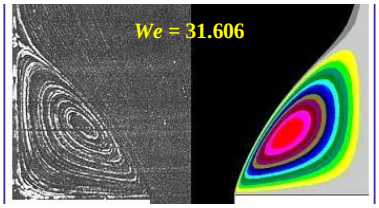


computational algorithms to numerically study these two disparate but equally important physical processes.

Mathematical modeling and simulation approaches are also used to study operations in polymer processing such as extrusion and injection molding. The rheology of long, linear and flexible polymer chains in molten state has been successfully modeled by the so called ‘reptation’ ansatz, whic h envisages snake-like Brownian motion of a chain within the confinement of a hypothetical tube that represents its surroundings.



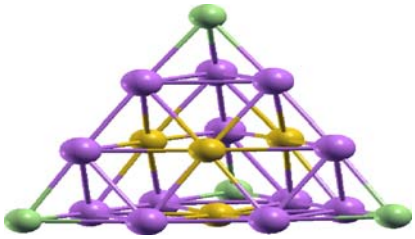




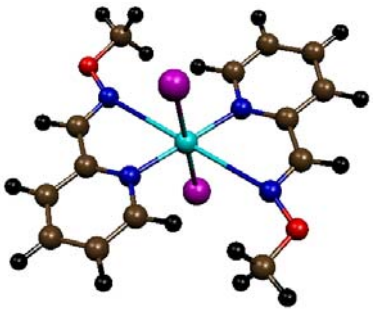
Such models are incorporated into specially developed finite element algorithms to simulate the processing-like complex flow of polymer melts, and validate simulations using experimental tools. This effort enables relating the coarse-grained molecular structure of a polymer to its engineering flow behaviour, which is ultimately important in ‘designing’ polymers to best suit a given processing application. Structure-property relations in polymers and colloids are also studied experimentally using a combination of rheology, home-built rheo-optics, X-ray and light scattering, microscopy and solid state NMR to understand polymer phase transitions, aggregation in colloids and organization of colloid-surfactant mesophases.

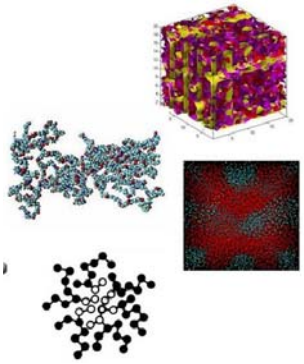
Advanced materials modeling

At the molecular and sub-molecular scale, a range of techniques ranging from ab initio methods to molecular dynamics have been employed to simulate material properties. These include relativistic coupled cluster methods, density functional methods, molecular dynamics and multi-scale simulations. In addition, estimating the thermochemical properties of a large number of organic free radicals has been made possible using a database of group-additivity values. Cheminformatics approaches are employed to estimate compound properties from structure data. A wide range of experimental and analytical facilities for synthesis and characterization of a variety of materials from nanoparticles to polymer films are also available.



Computational chemistry methods such as density functional theory (DFT) investigate phenomena at the sub-nano level – the level where the laws of quantum mechanics operate. Such methods can be applied to a variety of different problems, such as ones relating to organometallic catalysis, biochemistry, studies of reaction mechanisms, the search for alternative fuels, hydrogen storage and the proper understanding of the relationship of structure and bonding of chemical complexes with their physical and chemical characteristics. DFT has shed light on many problems relevant to Industry, specifically in the area of organometallic homogeneous and heterogeneous catalysis.





Another research area uses multiscale simulation of materials and bio-molecules, and quantum chemical calculations on low dimensional nano-materials to find out structure property relations, optical and electronic properties. Multiscale simulation of fuel cell polymer membranes: quantum chemical and molecular dynamics simulations to understand proton transfer mechanism and coarse grained dissipative particle dynamics simulation in mesoscale to elucidate the morphology of the membrane help establish the relation between morphology and proton transfer. Atomistic Molecular Dynamics (MD) simulations can explore the phase space of many-body systems on the sub-microsecond time and on the nanometer length scales. In order to carry out MD simulations, potentials (force fields) are required. Ongoing work on developing these force fields from chemical and structural description of molecules aims to calculate these parameters for new molecules. One of the current applications of MD simulations currently carried out in NCL is in the areas of protein aggregation diseases such as Alzheimer's, Parkinson's and Huntington's disease. Significant conformational changes and a host of other environmental factors precede protein aggregation. Developing a molecular level understanding of such phenomena can be key to preventing or reversing the symptoms of this class of debilitating diseases. Another area is the study of protein translocation through membranes. A biological membrane is a lipid bilayer with a hydrophobic interior and a hydrophilic surface. The conformations, interactions and the energetics of newly synthesized proteins or cleaved segments of membrane integrated proteins in traversing such a hydrophobic gradient can offer answers to a number of biological puzzles. In addition to the interactions between various parts of the macromolecule, structure and function are inextricably linked to the dynamical properties of the solvating environment. Characterizing the extent of this interdependence, distinguishing the contributions of different biomolecular entities in integrated biosystems, and trying to devise ways of indirectly modulating biomolecular function through the solvating environment are some aspects that are studied at NCL through MD simulations.

Student life@NCL

NCL has a vibrant group of almost 800 students engaged in postgraduate research. This greatly enhances the quality of the research atmosphere as there is great diversity both in terms of the individual background and interests, as well as research areas. There are formal student events such as the Science Day events, the student festival, in addition of course to the informal interactions at the local watering holes- the canteens, the shopping complex snack shops and the area cafes. Students are welcome to join the staff club, whose benefits include access to a library, sports facilities (badminton, bridge, tennis) and a weekly movie at the open air theater.

Residential facilities

Hostels

NCL hostels are of 3 types- Golden Jubilee (GJ), New Hostel and Scientist Apartments (SA). The GJ hostel is divided into 6 wings, 5 wings for boys and one wing for girls, with 12 rooms per wing on average. Each room is shared by 2 students. Hostel has its own dining facility (managed by students), TV room, and Gymnasium. The New Hostel contains 10 married-student suites and 10 rooms for unmarried research scholars, with 2 people sharing each room. For married students, one suite is allotted per student. In SA, 4 persons are sharing each SA, which has two rooms. For married people one suite is allotted per student. In case NCL accommodation is not available, temporary rental housing is available at Panchawati and other neighboring areas. Please contact current students for latest availability details. Typically deposit + 2 months rent is to be paid at the beginning. The cost is approximately 5000-35000 for deposit and 6000-10000 per room depending on the area and type of housing.

Apply for hostel as soon as possible after obtaining the ID card. Write a letter requesting accommodation. The letter should contain the ID number, joining date, marital status, and type of hostel requested. Under normal circumstances, all PGRPE students can expect to stay in on-campus accommodation. However all accommodation decisions are taken by the appropriate Student Academic Office or Administration authorities.

Food

NCL has two Cafeterias or canteens. The New Canteen is open on weekends in addition to working days. The old canteen serves tea, snacks and lunch at fixed times during working hours, and the new canteen serves snacks throughout the day except for lunch and dinner hours on all the days that it is open (between 8:30 am and 8:30 pm). Please note that canteen facilities are meant for the use of NCL staff and students only, and the consumption of non-canteen food in canteen premises is not allowed. Hostels have their own mess facilities.

Medical facilities

NCL has a health center with three doctors and basic lab facilities. Students may avail of this facility free of cost. In addition, students undergoing treatment in approved CSIR hospitals can get reimbursed for most expenses. Kotbagi hospital in Aundh is the nearest approved hospital.

NCL Surroundings

NCL is part of a vibrant community which includes a diverse set of institutions from the Defence research labs to the University of Pune, as well as commercial and residential areas of Baner, Pashan and Aundh. IISER Pune, NCL Innovation Part, and the Venture center and located on contiguous campuses. Links to several external sites with information can be found at http://www.ncl-india.org/aboutncl/showfileinvisit.jsp?mid=2

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