Multiscale Modeling and Simulation of Heterogeneous Catalytic Reactors
(8-12 January,2018)
Department of Chemical Engineering,NITwarangal

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1. Overview:

Mathematical modeling of diverse chemical processes running in various reactors can help to reduce experimental efforts during chemical process development. In heterogeneous catalytic reactors modeling of physico-chemical processes are represented as space-time hierarchical structures. The space scale ranges from 10^{-11} to 10^{3} m, the associated time scale ranges from 10^{-15} to 10^{8} s. The hierarchical multiscale approach is a backbone of the mathematical modeling of heterogeneous catalytic reactors. This approach consists in decomposing a complex chemical-technological process into chemical and physical components, studying these components independently and subsequently carrying out the synthesis of a general mathematical model from the models of separate parts of a complex process. Atomic-molecular processes and heat- and mass transfer in porous catalyst pellets or in the catalytic layer represent the lower two scales of the mathematical models of heterogeneous catalytic reactors. The processes of heat- and mass-transfer in the reactor, i.e. in the catalyst bed or monolith channel, represent the third scale, and modeling of a switch device with regard to the processes of mixing, heat exchange, etc – the forth scale. A multiscale mathematical model can describe the preceding levels and given level simultaneously.The present course is designed with the aim:

1. to consider a strategy for both one scale and multiscale EO-based modeling and simulation of heterogeneous catalytic reactors:

- ✓ to use the models with the elements that are needed, but without extra embellishments. This condition for a large class of reactors permits the model to be presented on each of the scales under consideration as a system of differential equations of dimensionality ≤ 2D with the first-order derivative with respect to a coordinate;
- ✓ to use an identical set of numerical tools such as integro-interpolation method, method of straight lines, a special case of a second-order Rosenbrock method, tridiagonal matrix algorithm or Thomas algorithm on each scale of a multiscale reactor model. Step size control is implemented with account for the rate of change of the variables on each scale. This efficient and robust algorithm significantly saves computation time and provides adequate accuracy and stability;

2. to demonstrate the EO-based modeling strategy at multiscale modeling of heterogeneous catalytic reactors such as tubular reactors, monolith catalytic reactor, and fluidized bed reactor

2. Objectives

The primary objectives of the course are as follows:

i. Expose the participants to space-time hierarchical structure of the models of physico-chemical processes in heterogeneous catalytic reactors,
ii. Expose the participants to the theory of the development of the reactor models with the elements that are needed, but without extra embellishments,
iii. Provide the participants with the theory of the numerical methods used for solution of the model equations,
iv. Building in confidence and capability amongst the participants in the application of the numerical tools,
v. Exposing the participants to the examples of using the EO-based modeling strategy at both one scale and multi scale modeling of heterogeneous catalytic reactors such as tubular reactors, monolith catalytic reactor, and fluidized bed reactor,

Dates	**8 - 12 January,2018**
Modules	• Introduction to Modeling and Simulation of heterogeneous Reactors • Heat and Mass transfer in the reactor • Numerical methods • EO-based modeling strategy at both one scale & multi scale
You Should Attend If…	▪ You are faculty member/research scientist / Industry professional working or interested in Modeling of heterogeneous reactors. ▪ You are technologist/engineer interested to learn numerical methods, EO-based multi scale modeling of heterogeneous catalytic reactors ▪ You are a UG/PG student or research scholar interested / working on heterogeneous reactors.
Fees	The participation fees for taking the course is as follows: **Participants from abroad: USD 300** **Participation from Indian Industry/consultancy firm: Rs. 5000** **Faculty (Internal and external) and Scientist: Rs. 3000** **Students & Research Scholars (with award of grade) :Rs1500** **Students (Without award of grade) :Rs 1000** The above fee includes all instructional material, computer use for tutorials and assignments, laboratory equipment usage, 24 h free internet facility. The participants will be provided accommodation on payment basis (subject to availability).

The Faculty

	**Dr.NadezhdaV.Vernikovskaya**is Seniorresearcher at Boreskov Institute of Catalysis SB RAS (BIC SB RAN), Novosibirsk, Russia, AssociateProfessor, Faculty of Natural Sciences, Novosibirsk State University (NSU), Novosibirsk, Russia and AssociateProfessor, Aircraft Faculty, Novosibirsk State Technical University (NSTU), Novosibirsk, Russia. Dr.Vernikovskaya has written approximately 100 peer reviewed journal articles, book chapters and conference papers. Most of her research has focused on modeling and simulation of heterogeneous catalytic reactors: Multiscale mathematical modeling of tubular reactors. Mathematical modelling of a fluidized bed reactor and structured catalytic reactor with short contact time for partial oxidation of methane and so on. For more details:https://www.researchgate.net/profile/N_Vernikovskaya, http://ciu.nstu.ru/kaf/persons/50366
	**Dr.Srinath Suranani** is currently Associate Professor in the Department of Chemical Engineering in the National Institute of Technology Warangal. His main areas of scientific research are Thermal conversion of solid waste, bio fuels, catalysis, micro reactors, Catalytic distillation, Process modeling and Simulation. He has completed three MHRD Sponsored R&D projects and presently executing R&D projects sponsored by ISRO & DRDO. Besides R&D projects, he has also involved in consultancy projects on simulation of process plantsand also filed three Indian patents. For more details: http://www.nitw.ac.in/faculty/id/16325/
	**Dr.Shirish Sonawane** is currently working as Associate Professor in Chemical Engineering Department National Institute of Technology Warangal, Telangana State, India. His research Interest focuses on synthesis of hybrid nanomaterials, cavitation based inorganic particle synthesis, Sonochemical synthesis of nanolatex. Process Intensification, Hybrid Waste water treatment system, Fuel Cells, Membrane separation processes. Dr Sonawane has published more than 80 research papers in reputed Journals, 7 book chapters, 6 Indian patent Applications. He was a recipient of prestigious BOYSCAST Fellowship from the Department of Science and Technology Govt of India. He worked in Particle Fluid Processing Center, University of Melbourne. He is also Heritage Fellow and worked in Chemical engineering department, InstitutoSuperioTechnico Lisbon Portugal. He has completed several sponsored R&D projects and consultancy projects. For more details: http://www.nitw.ac.in/faculty/id/16328/

Course Coordinators

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