

Overview of the Course

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 multi scale 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 fourth of a 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 multi scale 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 $\leq 2D$ with the first order derivative with respect to a coordinate;

- ✓ to use the 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 multi scale modeling of heterogeneous catalytic reactors such as tubular reactors, monolith catalytic reactor, and fluidized bed reactor.



Dr. Nadezhda V. Vernikovskaya is a Senior researcher at Borekov Institute of Catalysis SB RAS (BIC SB RAN), and Associate Professor, Faculty of Natural Sciences, Novosibirsk

State University (NSU), Novosibirsk, Russia. She 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 for various processes. Mathematical modeling of a fluidized bed reactors, modeling of structured catalytic reactor with short contact time for partial oxidation of methane and so on.

For more details:
www.researchgate.net/profile/N_Vernikovskaya
<http://ciu.nstu.ru/kaf/persons/50366>

Who can participate?

- This program is open to the Faculty, UG, PG students, and Research Scholars working or interested in Modeling of heterogeneous reactors from various Institutes.
- Engineers / Scientists working in Industries, Interested in learning numerical methods, EO -based multi scale modeling of heterogeneous reactors can also participate.

How to Register?

Stage-1: Web Portal Registration:

Visit <http://www.gian.iitkgp.ac.in/GREGN/index> and create login User ID and Password. Fill up the registration form and complete web registration by online payment of Rs. 500/-. This provides the user with life time registration to enroll in any number of GIAN courses offered.

Stage-2: Course Registration:

Login to the GIAN portal with the user ID and Password already created in Step 1. Click on Course Registration option at the top of Registration form. Select the Course titled "Multiscale Modeling and Simulation of Heterogeneous Catalytic Reactors" from the list and click on save option. Confirm your registration by clicking on Confirm Course.

Registration Fee:

Faculty & Scientists	Rs. 3,000/-
Participants from Industry / Consultancy firm	Rs. 5,000/-
Students & Research Scholars	
• Without award of Grade	Rs. 1,000/-
• With award of Grade	Rs. 1,500/-
Students from abroad	\$ 300

Boarding & Lodging Fee:

Faculty, Participants from Industry /Research Organizations	Rs. 4,000/- Accommodation -Visitors Block
Student & Research Scholar	Rs. 2,500/- Accommodation -Institute Hostel

Selection and Mode of Payment

Selected candidates will be intimated through e-mail. They have to remit the necessary course fee (**Mandatory for all**) and boarding & lodging fee (**if boarding & lodging is required**) to the Bank as per the details given below.

Account Name	GIAN NITW
Account No.	62447453600
Bank	State Bank of India
Branch	REC Warangal (NIT Campus)
Branch Code	20149
IFSC	SBIN0020149
MICR Code	506002030
SWIFT Code	SBININBB

Candidates registering early will be given preference in short listing process

For any queries regarding registration of the course, please contact the Coordinators:

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About GIAN Course

MHRD, Govt. of India has launched an innovative program titled “Global Initiative of Academic Networks (GIAN)” in higher Education, in order to garner the best international experience. As part of this, internationally renowned Academicians and Scientists are invited to augment the Country’s academic resources, accelerate the pace of quality reforms and elevate India’s scientific and technological capacity to global excellence.

About the Institute and Warangal

National Institute of Technology, Warangal (NITW) formerly known as RECW is the first among seventeen RECs set up in 1959. Over the years, the Institute has established itself as a premier Institution in imparting technical education of a very high standard, leading to B.Tech, M.Tech and Ph.D. programmes in various specializations of Science and Engineering streams. Warangal is known for its rich historical and cultural heritage. It is situated at a distance of 140 km from Hyderabad. Warangal is well connected by rail and road. National Institute of Technology, Warangal campus is 2 km away from Kazipet railway station and 12 km away from Warangal railway station.

About the Department

The Department of Chemical Engineering was established in the year 1964 and celebrated Golden Jubilee year in 2014. The Department offers B.Tech in Chemical Engineering, two M.Tech programmes (each in Chemical Engineering and Process Control) and Ph.D programs. Currently, the Department has 15 faculty members with different research expertise. The Department has good research facilities for both experimental as well as simulation based research.



A Five Day
GIAN Course on

Multiscale Modeling and Simulation of Heterogeneous Catalytic Reactors

January 8 - 12, 2018

Call for Registration and Participation

International Faculty

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