Integration of Molecular Design to Process Simulation for the Development of Industrial Chemical Products and Processes

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Overview

The main aim of the course is to introduce the fundamentals and practical applications of an emergent discipline in Chemical Engineering field: The multidisciplinary integration of computational tools of molecular and process simulation for the conceptual design of new products and process in the chemical industry.

Currently, lots of R & D departments of chemical companies present multidisciplinary teams of experts in different fields (theoretical chemists, physics, chemical engineers, etc.) applying computers and simulation tools to the development of new commercial products, procedures or processes, with the objective of minimizing the time and expenses investment. This course –taught by academics, researchers and practitioners experts in different simulation methods- is organized in three thematic sessions, concerning the simulation of chemical phenomena occurring at different time and length scale in the chemical supply chain: I) Quantum chemical methods for the design of atomic and molecular systems; II) COSMO-based methods for the prediction of thermodynamic properties of fluids and chemical mixtures, as key parameters to design separation and reaction industrial units; and III) Process simulation tools to model, integrate and optimize the unit operations involved in a chemical process. Each Session will include both theoretical classes to introduce the fundamentals of theoretical methods and practical classes to introduce the use of professional software applied in molecular, product and process design.

The successfully combination of currently available professional tools in different fields of chemistry open new opportunities of development for Chemical Engineers. This course presents a computer-aided multiscale research strategy for the conceptual design of new chemical products and process in the Chemical Industry, based on the successfully integration of well-founded and largely applied simulation methods in different disciplines of Chemistry.

Modules	**A. Quantum Chemical Methods and Molecular Design** **B. COSMO-based Methods and Product Design** **C. AspenPlus and Process Design** **All the modules will be held from December 12 - December 17,2016** **Number of participants for the course will be limited to fifty.**
You Should Attend If…	▪ Exposing participants to the fundamentals and the application of simulation methods in different fields of Chemistry. ▪ Demonstrating the main contribution of the integration of computational tools - used to simulate chemical phenomena occurring at different time and length scales- with the aim to design new chemical products with required properties for specific application. ▪ Providing exposure to practical problems and their solutions in the conceptual design of new chemical processes by using a computer-aided multiscale research strategy, as preliminary stages of project development
Fees	The participation fees for taking the course is as follows: **Participants from abroad : US $500** **Industry/ Research Organizations: INR 30000** **Academic Institutions: 10000** The above fee include all instructional materials, computer use for tutorials and assignments, laboratory equipment usage charges, 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

The Faculty

Dr. Jose Palomar is Associate Professor in Chemical Engineering Section of Universidad Autonoma de Madrid (Spain).His research interests include integration of molecular and process simulation computational tools for the conceptual design of industrial applications based on Ionic Liquids.

Dr. Tamal Banerjee is an Associate Professor at Department of Chemical Engineering, IIT Guwahati. His interest primarily lies in the Phase Equilibria Properties of Ionic Liquid systems and focuses on the use of Ionic Liquids (ILs)/Deep Eutectic Solvents (DES) as green solvents for various applications concerning both energy generation and environment mitigation.

Course Co-ordinator

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