UNH Materials Science Seminar

13:10-14:00, Wednesday, September 23, 2009
Kingsbury Hall N343
University of New Hampshire

Heterogeneous reaction systems: from molecular modeling to reactor optimization

Prof.dr. Olaf Deutschmann

Institute for Chemical Technology and Polymer Chemistry,
Universität Karlsruhe (TH), Karlsruhe Institute of Technology,
Kaiserstraße 12, 76128 Karlsruhe, Germany

Understanding and optimization of heterogeneous (gas-solid) reactive systems require the knowledge of the physical and chemical processes on a molecular level. In particular at high temperatures, at which reactions occur on the solid and in the gas-phase, the interaction of transport and chemistry becomes important. It will be shown how the understanding of the chemical and physical processes on a molecular supports the design and optimization of chemical reactors and processes following an approach of hierarchical models reaching from quantum mechanical simulation to Computational Fluid Dynamics. Furthermore, the coupling of two- and three-dimensional reactive flows including complex chemical reaction networks with mathematical optimization algorithm and their benefit for the solution of reaction engineering problems will be discussed. Applications will cover synthesis of hydrogen from logistic fuels, solid-oxide fuel cells, and carbon/carbon composites.

Prof.dr. Deutschmann currently holds the Chair of Chemical Technology at Universität Karlsruhe. He received an MS in Physics from University of Magdeburg and his PhD in Chemistry from University of Heidelberg, followed by postdoc research at University of Minnesota and Los Alamos National Lab. His research interests include energy-related and environmental catalysis, SOFC, CVD, combustion, modeling and simulation

Host: Professor Igor Tsukrov x2086