Catalytic Reaction Engineering of Exhaust After-treatment Systems

Professor Vemuri Balakotaiah Department of Chemical and Biomolecular Engineering University of Houston, Houston, Texas 77204-4004

Catalytic reactors, such as the three-way converter (TWC), diesel oxidation converter (DOC), lean NOx trap (LNT), selective catalytic-reduction reactor (SCR) and the diesel particulate filter (DPF), used in the treatment of exhaust gases from gasoline and diesel engines, are the most common man-made reactors (along with IC engines), with over one billion units in use. As in the case of most catalytic reactors, the performance of these units depends on the chemistry and interactions between the various catalytic components at the crystallite (nanometer) scale, the diffusion of reactants and products thorough the porous washcoat (micron scale), the momentum, heat and mass transport processes in the monolith channels (mm scale) and the speed and width of various concentration and temperature fronts along the monolith bricks (cm to meter scale). However, unlike the traditional catalytic reactors in large scale processes (e.g. ammonia or Fischer-Tropsch), the after-treatment reactors are multi-functional, work under highly transient conditions and their performance needs to be optimized in real time (for better fuel economy and emissions constraints). In the first part of this talk, I present an overview of various catalytic after-treatment units from a catalysis and reaction engineering point of view. In second part, I present reduced order models of such systems that incorporate the processes occurring at all scales but simple enough so that they can simulated in real time or faster than real time. Experimental validation, extension and possible use of such reduced order models for real time control and on-board diagnostics (OBD) in automobiles will also be discussed.



Dr. Vemuri Balakotaiah (Bala) is a Professor of Chemical and Biomolecular Engineering and Hugh Roy and Lillie Cranz Cullen Distinguished University Chair at the University of Houston. His research interests are broad and include the areas of chemical and catalytic reaction engineering, multiphase flow, transport in porous media and applied mathematics. He has published over 200 refereed articles, taught over 15 different courses and served as advisor/co-advisor to about 50 doctoral students in these areas.

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