Multi-Scale Modelling of Structured Catalytic Reactors

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As the power of computers increases, and software becomes more sophisticated, advanced computational modelling is being increasingly used in many chemical engineering processes. including the modelling of heterogeneous catalytic reactors. If we disregard empirical type models, then the most common technique used to develop a computational reactor model is to develop the partial differential equations (PDE) that describe the conservation equations. Together with relationships for kinetics and physical properties, the PDE can be solved by the appropriate numerical method, usually the finite volume (FVM) or finite element (FEM) methods. Commercial software is often used.

The physical and chemical phenomena that are important in a catalytic reactor happen at several length scales. A model of a heterogeneous catalytic chemical reactor thus represents a multi-scale problem. The smallest scale that might be considered is the molecular scale, where the various molecules interact with active sites to effect the reaction. It is certainly common to eliminate this scale through the use of global kinetic expressions, however, it is often necessary to use more detailed mechanisms, either because the global approach lacks accuracy or a more detailed description of the product distribution is desired. A typical porous catalyst has a pore scale on the dimensions of nano-metres, and the catalyst itself may consist of particles ranging in size from microns to millimetres. The void space inside the reactor is also typically on the millimetre scale, and the reactor itself may have dimensions on the scale of metres. To solve the governing PDE for the reactor requires the spatial discretization of the solution domain, however, a complete discretization of all scales is either extremely time consuming or not possible at all. Usually only the largest scale is discretized and some form of volume averaging is used over the domain. The challenge is to incorporate the smaller scale information in the large scale model. This is usually done using sub-models, referred to generically as scale bridges. Scale bridges can be as simple as an algebraic equation or require the solution of a complex set of PDE on a sub-grid. The efficient choice of a scale bridge is often crucial to achieving a cost effective and timely solution.

This talk will discuss some methodologies for hierarchical multi-scale model reduction. It will focus on the use of pre-computed data stored in look-up tables as a means of achieving said computational efficiency. Some practical examples used in the modelling of structured reactors will be illustrated.

Professor R.E. (Bob) Hayes is a Professor of Chemical Engineering at the University of Alberta. He has been active in Catalysis since his undergraduate years. Following a B.Eng. earned at the Technical University of Nova Scotia (TUNS), he pursued a PhD with Professor John Thomas at the University of Bath, UK. He continued his work on catalysis at TUNS as an Assistant Professor, studying the methanation reaction, before moving to the University of Alberta in 1985. Since 1990, he has worked in the area of catalytic combustion in structured catalytic reactors, both for the mitigation of fugitive methane emissions and in the development of automotive catalytic converters. The research work has been conducted in collaboration with both industrial and governmental laboratories, as well as with colleagues and other Canadian and International Universities. He is the author or co-author of over 100 scientific papers and six textbooks, including the reference work, *Introduction to Catalytic Combustion*, published in 1997, and is co-author of the historical fiction novel *Riot and Retribution*.

His current research interests include catalyst development for the low temperature oxidation of methane in lean and wet gas streams, kinetic and reactor modelling of automotive exhaust gas after treatment systems and catalytic distillation for the production of biofuels.