MULTI-MODE LOW-DIMENSIONAL MODELS FOR REAL TIME SIMULATION OF CATALYTIC AND MULTIPHASE REACTORS

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As the length and time scales associated with continuum models of catalytic and multi-phase reactors vary from the molecular to the macro scale, for most cases of practical interest, even with the present computing power, it is impractical to solve such detailed models and explore all the different types of solutions that exist in the multi-dimensional parameter spaces. Accurate low-dimensional models that retain the multiscale physics and expressed in terms of measurable variables are desired for the purpose of design, control and optimization of these systems in real time.

We have recently shown that the Liapunov-Schmidt (L-S) technique of bifurcation theory is also an excellent multiscale averaging technique for reactor models described by coupled nonlinear partial differential equations (PDEs) of diffusion-convection-reaction (DCR) type. This procedure starts with detailed DCR models and takes advantage of the separation of the length or time scales to reduce the spatial and/or temporal degrees of freedom and to obtain multi-mode multiscale low-dimensional models in terms of measurable quantities such as cup-mixing concentrations or temperatures. This procedure is rigorous and is equivalent to the Taylor expansion of a detailed fundamental model in terms of one or more small parameters representing separation of length/time scales in the original model. In such an expansion, the lowest order term is the conservation law at the macroscale while higher order corrections modify it by including the physical phenomena at smaller and smaller length scales.

In the first part of this talk, we illustrate the application of the L-S technique by deriving multi-mode multiscale low-dimensional models for various types of catalytic and multi-phase reactors described by DCR models. For some selected cases, we determine the accuracy of these low-D models by comparing their solution with that of the full PDEs model. We also show that the low-dimensional models derived by the L-S technique are hyperbolic in nature and hence retain the proper physics (especially in convection dominated systems), in contrast to the traditional parabolic models that may lead to some physical inconsistencies. Further, we show that the hyperbolic models are more convenient and speed up the numerical computations compared to the traditional parabolic models. In the second part of the talk, we illustrate the application of the low-D models for real time simulation and control of exhaust from gasoline and diesel engines.