413a Multiscale Averaging Methods for Diffusion-Convection-Reaction Models

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Due to the fact that the length and time scales associated with continuum models of diffusion-convection-reaction (DCR) type vary from the molecular scale to the macro or process scale, for most cases of practical interest, even with the present day computational power, it is impractical to solve such detailed models (consisting of several nonlinear PDEs) 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. We have recently shown that the Liapunov-Schmidt (L-S) technique of classical bifurcation theory is an excellent multiscale averaging technique for DCR models described by coupled nonlinear PDEs. This procedure starts with detailed models based on the fundamental laws and takes advantage of the separation of the length or time scales (expressed in terms of one or more small parameters in the dimensionless form of the model) to reduce the spatial/temporal degrees of freedom and to obtain multi-mode multiscale low-dimensional models in terms of measurable quantities (such as cup-mixing concentrations). This procedure is rigorous and is equivalent to the Taylor expansion of a more 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 simplified model while higher order corrections modify the model by including the physical phenomena at smaller and smaller length scales. In this work, we extend the L-S technique to include DCR models with more general boundary conditions (Dirichlet, Periodic and Robin) as well as examine the convergence and accuracy of the method by applying it to some model problems and comparing the solutions of the averaged models to those of the full PDEs. We also derive multiscale averaged models for various applications in the areas of catalytic reaction engineering, multiphase reactors, reactive dissolution of porous media and biomedical reaction engineering.