224b Development of a Multiscale Scheme for Modeling Fluid Phase Concentration Variations in Two Dimensions for Catalytic Flow Reactors

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Although a small number of models have been developed in the past for designing reactors employing heterogeneous catalysts which link a molecular-level solver for the catalyst phase with a macroscopic scale solver for the fluid phase, [1-4] they have not included variation in fluid phase concentrations in contact with the solid phase. This is mainly because of the huge computational expense involved in solving a catalyst domain large enough to experience a concentration variation in the contacting fluid. However, for a considerable number of catalytic flow reactor configurations such as monoliths, a model which can solve the fluid phase concentration variations in two dimensions would be valuable. Recently, with the development of advanced multiscale methods such as patch dynamics, [5-7] it is possible to conceive a strategy for developing such models.

In the present work, a multiscale hybrid approach that couples continuum descriptions of thw fluid phase and kinetic Monte Carlo simulations of the catalyst domain was developed. A number of catalytic domains, placed as patches along the length of the reactor, were solved using kinetic Monte-Carlo (kMC) and linked with a finite difference (FD) solver for the fluid phase. Patch dynamics concepts such as lifting, restriction and interpolation were employed to provide the complete set of boundary conditions to the continuum solver. A simple kinetic mechanism involving adsorption, desorption and a single-step surface reaction was used to compare the solution obtained using this scheme with a model involving a wholly implicit solution. The effect of different parameters involved in coupling kMC with the FD scheme and the application to more rich chemical mechanisms will be discussed.

References: [1] Vlachos, D. Multiscale integration algorithms for homogeneous-heterogeneous reactors. AIChE J. 1997. 43(11), 3031–3041. [2] Lam, R.; Vlachos, D. Multiscale model for epitaxial growth of films: Growth mode transition. Phys. Review B 2001. 6403, 396–404. [3] Lou, Y.; Christofides, P. Estimation and control of surface roughness in thin film growth using kinetic Monte-Carlo models. Chem. Eng. Sci. 2003. 58, 3115–3129. [4] Rusli, E.; Drews, T.; Braatz, R. Systems analysis and design of dynamically coupled multiscale reactor. Chem. Eng. Sci. 2004. 59, 5607–5613. [5] Kevrekidis, I.; Gear, C.; Hyman, J.; Kevrekidis, P.; Runborg, O.; Theodoropoulos, C. Equation-free multiscale computation: Enabling microscopic simulators to perform systemlevel tasks, 2002. Submitted to Comm. Math. Sci., physics/0209043 at arxiv.org. [6] Gear, C.; Kevrekidis, I. Boundary processing for Monte Carlo simulations in the gap-tooth scheme., 2002. Physics/0211043 at arxiv.org. [7] Gear, C.; Li, J.; Kevrekidis, I. The gap-tooth method in particle simulations. Phys. Lett. A 2003. 316(3), 190–195.