Stochastic Hybrid Multiscale Model for Gas-Solid Interfacial Systems

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Through a concurrent coupling approach based on domain decomposition, we develop a stochastic multiscale simulation method for heterogeneous catalytic systems at the micron or submicron scale. We employ kinetic Monte Carlo (KMC) to accurately describe complex reaction mechanisms on the catalytic surface, whereas we use fluctuating hydrodynamics (FHD) to effectively describe transport behavior in the bulk gas region. The surface KMC model is a stochastic particle dynamics model, which can resolve lateral interactions among adsorbates on the catalytic surface. While these interactions have been proven to significantly affect surface chemical reactions, mean-field descriptions such as the microkinetic model by nature fail to describe them. In our coupling approach, this KMC model is then interactively coupled with continuum dynamics at the mesoscale so that the fidelity of both parts of the simulation can be significantly enhanced. Since mass, momentum, and energy fluxes from particle dynamics are by nature stochastic due to intrinsic thermal fluctuations, the use of FHD for the continuum counterpart is essential. Under the reasonable assumption that interactions between the gas and surface phases occur only through adsorption and desorption processes, we construct a flux-based coupling of KMC and FHD by modeling these processes and defining how to update each phase accordingly. Based on the Langmuir model of adsorption, we develop a Markov process modeling of adsorption and desorption processes, through which discrete (Poisson) fluctuations in KMC and continuous fluctuations in FHD are incorporated. Via physically correct exchanges of instantaneous fluxes, both parts of the simulation are consistent with statistical mechanics, which ensure correct nonequilibrium descriptions. We present a mathematically and physically sound coupling strategy and a corresponding numerical scheme. We also showcase our high performance computing (HPC) implementation using an established KMC model for the CO oxidation on metal surfaces.