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# Development Of A Filtered Reaction Rate Model For Coarse-Grid Simulations Of Reactive Gas-Solid Flows

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## Extended Abstract

Reactive gas-solid flows are commonly encountered in many industrial processes. In reactive gas-solid flows, the inhomogeneous mesoscale structures stemming from the interphase interaction and transport behavior considerably affect the overall fluid dynamic, transport and reaction behavior [1]. However, the flow, mass transfer and reaction in reactive gas-solid flows span a wide range of spatial-temporal scales, and it is computationally difficult to describe and predict the fluid and particle dynamics in detail in industrial-scale reactors. Thus, coarse-grid simulation, which can simulate industrial-scale reactors, is widely used. It should be noted that such coarse-grid simulations do not fully resolve these inhomogeneous structures, which can cause the overprediction of the reaction rate [2]. Therefore, the sub-grid correction of the microscopic reaction rate model is required in coarse-grid simulations. The aim of this work is to simulate and analyze the effects of mesoscale structures on reaction behavior and construct a reasonable filtered reaction rate model. MFiX software was used to simulate a series of high-resolution fine-grid simulations of isothermal, solid-catalyzed surface reactions with a power law reaction rate in periodic systems. The averaged solid volume fractions of the computational domain for the considered different reaction kinetic models are 0.05, 0.10, 0.30 and 0.50, the intrinsic reaction rate constant ranges from 6.15 to 615.4(1/s), and the reaction orders of the power law reaction are 0.5, 1 and 2. Then the simulation results are analyzed using the filter technology, conditional average and correlation analysis, which have been widely used in mesoscale drag and heat transfer coefficient modeling [3-5]. The results show that the Damköhler number (the ratio of the specific surface chemical reaction rate to the mass transport rate to the reaction surface), solid volume fraction and filter size are significantly related to the mesoscale reaction rate. A filtered reaction rate model suitable for coarse-grid simulations is constructed. We find that the dependence of the correction factors for the new model on the Damköhler number for different reaction kinetic models is invariant with the reaction order at the same solid volume fraction and filter size. In general, the correction factors for the new model retain an inverted bell-shaped dependence on the solid volume fraction and it approaches unity at the very dilute/dense regions. The new model was evaluated by simulating the reaction behavior of the circulating fluidized bed for ozone decomposition. Furthermore, the extension for the filtered reaction rate model to the reactive gas-solid systems with the expansion and contraction effect is considered. The effects of the expansion and contraction on the filtered reaction rate model are studied, and the possibility of correcting the model by using the surrounding solid volume fraction, gas phase density gradient, velocity divergence, Reynolds number based on slip velocity, and other variables as new markers are explored. After a series of new fine-grid simulations and data analysis, the filtered reaction rate model was further corrected, and a more well-adapted and accurate filtered reaction rate model was obtained. A prior test shows that the filtered reaction rate model based on fine-grid simulations can get better prediction results in the coarse-grid simulations.

**Keywords:** Reactive gas-solid flows, Fluidization, Mesoscale structures, Filtered reaction rate model

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