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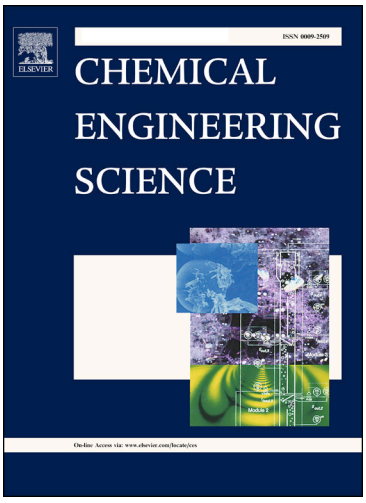

Direct Numerical Simulation of Fluid Flow and Mass Transfer in Dense Fluid-particle Systems with Surface Reactions

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Direct Numerical Simulation of Fluid Flow and Mass Transfer in Dense Fluid-particle Systems with Surface Reactions

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Abstract

In this paper, an efficient ghost-cell based immersed boundary method is introduced to perform direct numerical simulation (DNS) of mass transfer problems in particulate flows. The fluid-solid coupling is achieved by implicit incorporation of the boundary conditions into the discretized momentum and species conservation equations of the fluid phase. Taking the advantage of a second order quadratic interpolation scheme utilized in the reconstruction procedures, the unique feature of this ghost-cell based immersed boundary method is its capability to handle mixed boundary conditions at the exact position of the particle surface as encountered in systems with interplay between surface reactions and diffusion.

A fixed Eulerian grid is used to solve the conservation equations for the entire computational domain. Following a detailed verification of the method in the limiting case of unsteady molecular diffusion without convection, we apply our method to study fluid-particle mass transfer for flow around a single sphere and a dense stationary array consisting of hundreds of spheres over a range of Damköhler numbers.

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