Multiscale two-dimensional multiparticle reactor model for non-catalytic gas-solid reactions

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Abstract

Non-catalytic gas-solid reaction systems encompass a range of industrial processes. Among them, the oxidation and reduction of metallic oxides or metals using hydrogen are increasingly applied as environmentally friendly technologies, such as Chemical Looping Hydrogen (CLH) production and Hydrogen Direct Reduction (H-DR) of iron ore (Chang et al., 2023; Zare Ghadi et al. 2020). Despite this, most existing simulations from the literature considerably simplify the transport and reaction phenomena involved at the particle scale (Zare Ghadi et al. 2020). In fact, the complex mathematical equation of such systems is derived from the transient characteristics of the solids that affect the local physical properties during the reaction. In this study, a multiscale model for non-catalytic gas-solid reactions was developed to evaluate the parameters that hierarchically affect process performance. The model considers the mass, heat, and momentum transport equations for the gas flow in a porous medium and the solid particles in counter-current flow, comprising the kinetic model of multiple non-catalytic reactions that occur inside the particles. The reactor and the solid particles are discretized based on the Finite Element Method (FEM), and an extra dimension is used to simulate the particle scale coupled to the reactor scale. The model was validated with industrial data, showing detailed profiles of gas and solid concentration, and temperature along the pellet radius at different reactor positions, as well as solid conversion, gas concentration, and temperature of both phases along the reactor. The multiscale model provides important information on non-catalytic solid reactions, allowing for the optimization of the performance of industrial-scale reactors.

Keywords

Non-catalytic reactions, multiscale simulation, hydrogen, direct reduction, finite element method.

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References

W. Chang, Y. Hu, W. Xu, C. Huang, H. Chen, J. He, Y. Han, Y. Zhu, X. Ma, X. Wang: Catalysts (13), 279, 2023.

A. Zare Ghadi, M. S. Valipour, S. M. Vahedi, H. Y. Sohn, steel research int. (91), 1900270, 2020.