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The interplay between temperature evolution, species distribution, and microstructure dynamic in a calcining porous particle

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Reacting particle systems play a crucial role in various industrial applications, with limestone calcination serving as a prime example. In this process, applying high-energy input to calcium carbonate ($CaCO_3$) particles results in the production of active lime solid (calcium oxide CaO) and the by-product carbon dioxide (CO_2) gas. The legal obligation to mitigate CO_2 emissions has a notable impact on production costs, emphasizing the need for a thorough understanding of the calcination process. Such an understanding can enhance conversion process efficiency and enable the achievement of desired CaO structures, crucial for high efficiency in CO_2 adsorption. This study introduces a pore network model to explore the interplay between intraparticle heat and mass transfer, pore structure changes during chemical reactions, and their interactions with the surrounding fluid-solid environment in a single particle. The pore space and solid skeleton of the particle are approximated as regular-lattice networks, incorporating cylindrical pores and volume-less nodes. Local reaction rates are determined based on the effective specific surface area and local CO_2 pressure. Thermal energy is supplied through hot gas flow convection at the network's surface. Solid element dimensions and corresponding pore structures are updated during each time step, enabling the tracking of temperature evolution, local conversion, and void space structure changes within the particle. Simulation results reveal that when the bulk gas has initially low CO_2 pressure, calcination extends beyond the particle surface and occurs within the particle. As a result, the released CO_2 becomes trapped due to internal mass transfer resistance, impeding further calcination. On the contrary, exposure to high initial CO2 pressure exclusively promotes local calcination reactions at the particle's surface. The initial bulk CO_2 pressure also has a notable impact on the final structure of CaO. This intricate interplay in calcination, as demonstrated by the simulations, provides valuable insights for a better understanding and optimization of industrial processes, applicable not only to calcination but also to other heterogenous reactive systems.

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