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Pore network modeling of calcination in single particles with evolving microstructure

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A pore network model for calcination of a single particle (made of magnesium carbonate) is developed in order to better understand and quantify the heat and mass transfer within the particle, morphological changes of its pore structure, chemical reactions and the connection to the particle's fluid-solid surrounding. Both the pore space and solid skeleton of the particle are approximated as regular-lattice networks. Local reaction rates are expressed by the one-step kinetic model using the classical Arrhenius equation with constant coefficients. Mass balance equations are set up to solid elements (i.e. magnesium carbonate and magnesium oxide) and carbon dioxide at pores. At each time step, the size of solid elements and complementary pore structures is updated. Using this pore network model, the development of the carbon dioxide profiles at the surface as well as at the reaction front where the decomposition reaction takes place are predicted over time. Though this model is oversimplified from point of view of physics and chemistry, it shall serve as an essential step to develop superior pore network models that can simulate calcination of a single particle at reaslistic process conditions.

Participation

In-Person

References

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