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Discrete pore network modeling of limestone particle calcination under non-isothermal conditions

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In this study, we present a discrete pore network model to simulate the coupled heat transfer, mass transfer, chemical reactions, and fluid-solid interactions during the calcination of a single limestone particle under realistic, non-isothermal conditions. By resolving intra-particle transport and reaction processes, the model captures internal temperature distributions through local energy equations, offering a detailed representation of the particle's thermally thick behavior. Unlike previous models, this approach systematically updates the solid grain sizes and pore structures over time, enabling precise tracking of local conversion profiles, pore size distributions, and internal temperature gradients. The interplay between heat and mass transfer leads to a non-uniform release and transport of CO_2 within the particle, with certain pore regions experiencing pressures that exceed equilibrium levels and result in pore clogging. These localized phenomena are critical for understanding the dynamic configuration of gas-particle interactions and their influence on macroscopic behavior. The insights gained from this model contribute to the development of advanced continuum models that incorporate closure strategies for unresolved gas-solid interactions, aligning with the overarching goal of enhancing predictive capabilities for thermochemical treatments. This work highlights the importance of intra-particle processes in the context of calcination and bridges the gap between discrete particle-scale models and larger-scale CFD/DEM descriptions, providing a pathway for improved modeling of high-temperature particle treatments under realistic industrial conditions.

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