Lattice-Boltzmann modeling of hydrate formation in brine

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Abstract

The characteristics of hydrate formation in brine are critical for understanding gas hydrate accumulation in deep-sea sediments and evaluating the removal efficiency of hydrate-based desalination. A numerical model based on Lattice Boltzmann method (LBM) is developed to study the process of hydrate formation in brine, in which the effect of salt ions on water activity and equilibrium temperature of hydrate formation are incorporated into the kinetic-reaction model. The model can capture the complex coupling between concentration gradient caused by removal of salt ions by hydrate formation and mass transfer related to the supply of guest molecule to the surface of hydrates, and describe the process of hydrate formation in brine by combining the improved kinetic-reaction model. The model is validated by a comparison with both analytical solution and experimental results and then used to study the process of hydrate formation in brine (see Fig. 1 below). The effects of initial concentration of salt ions on hydrate formation by quantitatively tracking water conversion and consumption of guest molecules are investigated.

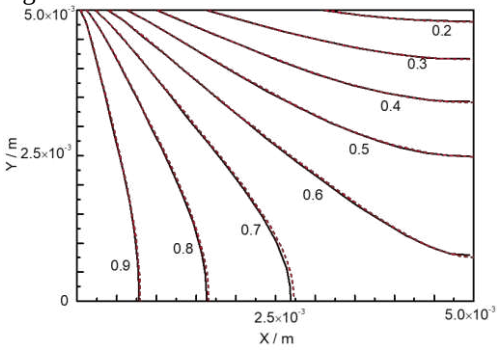

Figure 1: Contour of steady-state concentration for Damkohler number=5. The solid lines and dashed lines are simulation results and analytical solution, respectively.

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