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Multiphase Reactive Transport Modeling of CO2 Dissolution in Geological Carbon Sequestration Using Lattice Boltzmann Simulations

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Geological carbon sequestration is the most suitable way to alleviate the negative influence caused by CO2 at the field scale. CO2 dissolution as one of the most indispensable and predominant trapping mechanisms is a complicated process involving both physical and chemical phenomena. In this work, CO2 dissolution after capillary trapping far away from the injection well under different environmental conditions is investigated to elaborate the main controlling mechanisms of CO2 dissolution reactions and the corresponding sensitivity analysis during these processes.

Coupled with homogeneous reactions in the brine and heterogeneous reactions at the CO2-brine interface, a multiphase Shan-Chen multiple-relaxation-time lattice Boltzmann model with multicomponent transport is established to capture CO2 dissolution reactions with phase transitions in saline aquifers. Controlling mechanisms of CO2 dissolution reactions are probed by estimating the temporal evolution of CO2(aq) concentration and the dissolved CO2 nodes under different diffusion coefficients and CO2 saturations in a periodic domain. Furthermore, CO2 dissolution in porous media is captured to explain the ion evolution during homogeneous reactions and characterize the impact of different factors, namely partial pressure, formation temperature and salinity, on this process in the view of practical application.

The rapid mass transport, namely the large diffusion coefficient, could keep the CO2(aq) concentration gradient at the scCO2-water interface at a high level, which would accelerate CO2 dissolution processes. The ratio of the equilibrium time between various cases is nearly about 3 times. Additionally, the reactive interfacial length also affects CO2 dissolution reactions. It can be concluded from the simulated results that higher reactive interfacial length would make the security of CO2 trapping greater under the same CO2 saturation. More importantly, it is found that the CO2 dissolution process is non-equilibrium and would not be omitted when the sequestration efficiency is estimated in reservoir-scale simulations. Otherwise, the accuracy of the results cannot be ensured. It is beneficial for sequestration efficiency to adopt the high-pressure region due to greater CO2 density and equilibrium concentration at the scCO2-water interface. Besides, the formation temperature, which should be prudently selected in the targeted saline aquifer for practical operation, has both positive and negative effects on CO2 dissolution. In terms of salinity, the more ion strength is the less trapping efficiency is.

This study offers not only a deeper understanding of multiphase reactive transport of CO2 dissolution in porous media during geological carbon sequestration but also a new idea about the same physicochemical backgrounds, such as the hydrogenation of levulinic acid.

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