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# Numerical simulation for the reactive multiphase flow in porous media during the Carbon Capture and Storage process

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In recent years, the extensive using of fossil fuels has led to a substantial release of greenhouse gases, resulting in a pronounced warming trend in the Earth's climate. To mitigate the process of global climate warming, Carbon Capture, Utilization, and Storage (CCUS) projects have gained prominence, with the efficient sequestration of CO2 into geological formations becoming a focal concern. In the process of CO2 sequestration, the permeation behavior of CO2 in water crucially determines its storage capacity and rate. On the one hand, the dissolution of CO2 in water increases the storage capacity. On the other hand, some rocks in the formation, such as glauberite, will dissolve under the combined action of carbon dioxide and water, thereby increasing the storage space of carbon dioxide. To comprehensively investigate the various influencing mechanisms in the CO2 sequestration process, pore-scale simulations offer an effective approach, allowing for a microscopic examination of mechanisms and a systematic analysis of influencing factors to further guide the sequestration of CO2. The lattice Boltzmann method, as a mesoscale approach, efficiently facilitates multiphase and multiscale coupling, enabling the treatment of complex solid-liquid/gas-solid boundary conditions. Thus, in this study, the lattice Boltzmann method was adopted for research purposes.

In this study, a new LB model was built to consider the effect of both CO2 dissolution in water and salt dissolution mechanisms on the CO2 storage process. What's more, the CST-LB model was adopted to describe the interfacial mass transfer, and the VOP method was used to update the structure of porous media. The impacts of factors such as wettability, salt concentration, and porosity on the CO2 sequestration process were comprehensively explored. The results indicate that, during the displacement and dissolution processes of CO2 in the aqueous phase, an increase in CO2 concentration in water leads to the gradual dissolution of some soluble salts in the solid phase. But there are some risks. While this expands the storage space for CO2, the dissolution of soluble salts results in the phenomenon of breakthrough points between CO2 and water, forming preferential channels that cause a substantial outflow of CO2. Additionally, when the wettability angle of the rock phase is greater, after CO2 displacement, some water remains in the porous medium, reducing the CO2 storage space and consequently diminishing sequestration capacity. This study provides crucial guidance for the sequestration of CO2.

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