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Enhanced CO2 Storage in Saline Aquifer by Electric Field Considering Formation Wettability

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Geological CO2 storage involves injecting captured CO2 into various geological formations, in which saline aquifers have the largest storage potential around the world. In the context of carbon neutrality, one of the key issues is to store CO2 as much as possible on the premise of formation stability. In this paper, we find that external electric field can enhance CO2 storage in saline aquifers. The different mechanisms of CO2 storage enhancement in hydrophobic and hydrophilic formations are revealed by molecular dynamics simulations. The following conclusions can be drawn. (1) In order to consider formation wettabilities, a carbon-based pore wall, a hydroxylated quartz pore wall and a calcite wall are constructed. CO2 tends to accumulate more readily on carbon-based wall, while H2O exhibits a higher tendency to accumulate near hydroxylated quartz wall and carbonate wall, indicating different wettabilities of the three walls. (2) On a short time-scale, CO2 is stored in adsorbed and dissolved states in saline aquifers of hydrophobic and hydrophilic formations. (3) In the absence of an electric field, the dissolved CO2 accounts for 42.50% in the hydrophobic formations; the adsorbed CO2 accounts for 12.4% in the hydrophilic quartz formations. When an external electric field is applied vertically to the wall, the proportion of dissolved CO2 in the hydrophobic formations increases to 63.23%; the proportion of adsorbed CO2 in the hydrophilic quartz formations increases to 21.76%. However, the external electric field has negligible effects in the hydrophilic carbonate formations. (4) The orientation of H2O molecules and the hydrogen bonds are further analyzed to reveal the different enhancement mechanism. In the hydrophobic formations, the external electric field induces oriented H2O molecules, leading to their preferential accumulation near the wall, rendering the initially hydrophobic wall hydrophilic, thereby reducing the available space for adsorbed CO2 and promoting its dissolution in the H2O phase. In the hydrophilic quartz formations, the external electric field drives H2O away from the surface, concurrently reducing the number of hydrogen bonds formed between H2O and the hydrophilic wall by approximately 24.22%. This reduction diminishes the hydrophilicity of the wall. In the hydrophilic carbonate formations, there are no hydrogen bonds between H2O molecules and the wall. Therefore, the electric field has negligible effects on the wettability of the wall and CO2 storage. This study proposes a novel technique to enhance CO2 storage in saline aquifers of different wettabilities by electric field. The molecular perspective revealing the enhancement mechanism is expected to provide theoretical guidance in the future practical application.
Keywords: Geological CO2 storage; electric field; molecular dynamics simulation;

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