

EGU22-6837

<https://doi.org/10.5194/egusphere-egu22-6837>

EGU General Assembly 2022

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Interfacial Tension of CO₂-Water Under Conditions for High-Temperature Geothermal Systems: Prediction and Investigation by Molecular Dynamics Simulation

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For several decades, research on CCUS (carbon capture, storage, and utilization) have been extensively carried out to achieve substantial reduction of the amount of CO₂ emitted into the atmosphere and effective resource development. In recent years, high temperature reservoirs have recently been considered as a target for CO₂ injection. This aims at development of unconventional geothermal resources and CO₂ mineralization.

Since the value of CO₂-water interfacial tension is a fundamental property of fluid behavior in CO₂-water-rock systems, many studies have been reported on CO₂-water interfacial tension. However, the temperature of the geothermal reservoir in the above-mentioned technology may be up to 300 °C, which is much higher than typical conditions for CCUS. It is not easy to perform measurements under such high temperature conditions, and no experimental data have been reported in existing studies.

Therefore, in this study, we performed molecular dynamics simulations to estimate the interfacial tension up to 300 °C, and also studied the detailed properties such as density and dynamics.