Molecular Dynamics Study on the Dynamic Contact Angle of CO_2/H_2O/Mineral System in Nano Pore Throat

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CO_2 Geological Storage (CGS) is one of the most promising technologies to reduce the amount of CO_2 emissions into the atmosphere. Enhanced oil recovery in addition to the sequestration in the geological formation has been actively studied, and these are considered to be a significant strategy for sustainable energy development. In order to conduct the project safely, it is necessary to predict and understand the sealing performance of the caprock. This is evaluated by the threshold value of the capillary pressure. This pressure is formulated as Young Laplace equation; the capillary pressure is proportional to $2\Gamma\cos\theta/a$. (Γ : interfacial tension between CO_2 and brine, θ : contact angle, a: radius of the pore throat) Water-receding contact angle, which is represents the wetting behaviors in the drainage process, should be evaluated. Therefore, there have been a lot of experimental measurements of the dynamic contact angle. However, there is no data in the nano scale, which is the actual scale of the caprock in the CGS site. CO_2 and H_2O confined in the nano pore throat is likely to behave in a different manner. This is because the effect of the surface forces working on the fluid phases from the mineral surface is much larger than those in the macroscopic systems.

Considering the importance of studying the wettability in nano scale and its difficulty in direct measurements, we calculated the contact angle by using molecular dynamics simulation. We obtained both advancing and receding contact angles. Moreover, we studied the shape of the interface both at meniscus and film regions, which have crucial roles in wettability alteration.

Keywords: CO2 Geological Storage, Wettability, Molecular Dynamics

