Molecular Dynamics Study on the Salinity Dependence of the Contact Angle of CO_2/Brine/Muscovite System

*Masashige Shiga[1], Yungfeng Liang[2], Sumihiko Murata[1], Weiren Lin[1]

1. Kyoto University, 2. The University of Tokyo

CO_2 geological storage is one of the technologies to reduce CO_2 emissions into the atmosphere. CO_2 is recovered from a large-scale source and is injected into deep underground and stored in the geological formation. By the function of the shielding layer on the upper part of the reservoir layer, it is possible to store CO_2 for a long term stably. The sealing performance of the caprock is evaluated by the capillary pressure acting on the void space of the mineral particles. Wettability of the fluid to the mineral surface directly affects the capillary pressure. It is evaluated by the contact angle, but it is complex and unknown in part because it is affected by the interaction of CO_2/Brine/Mineral three phases. The contact angle can vary depending on various factors such as temperature, pressure, and the type of mineral. Arif *et al* (2016) experimentally measured the salinity dependence of the contact angle of CO_2/Brine/Muscovite system. The results showed that the contact angle increased by increasing salinity. This trend can possibly lead to the decrease of storage capacity and sealing performance.
In this study, the contact angle is calculated by using molecular dynamics calculation, and the mechanism of the contact angle change is discussed, focusing on the structural change of the thin film on the muscovite.

Keywords: CO2 Geo Sequestration, Wettability, Molecular Dynamics

