Development and Validation of Molecular-based Models for the Prediction of Thermodynamic and Transport Properties of CO$_2$–Brine Mixtures

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Emissions of long-lived greenhouse gases (GHGs) are believed to be a major driver of climate change. Carbon dioxide (CO$_2$) is the most important greenhouse gas, according to the latest available studies, and one of the most prominent strategies to lower its emissions is carbon capture and sequestration (CCS). CO$_2$ can be stored in geological repositories, such as hydrocarbon reservoirs in which sodium chloride (NaCl) is the most common dissolved salt. For the optimum design of any CCS process, accurate experimental data and computational models are necessary to provide reliable prediction of primary and derivative thermodynamic properties as well as transport properties. Despite the increasing importance of CCS processes, the lack of reliable physical property data cause significant uncertainties and create barriers toward the optimum design of the process. This study focuses on generating and validating molecular-based models and methodologies to allow for reliable prediction of the thermodynamic and transport properties of CO$_2$–brine mixtures over a broad range of temperatures and pressures relevant for geological storage.

Atomistic simulations can be a valuable tool to complement experimental measurements of transport and thermodynamic properties. An advantage of the molecular dynamics (MD) and Monte Carlo simulation methods, compared to the macroscopic models, is that they can give insight to the systems at the molecular level. This approach has become more popular in recent years thanks to the significant increase of computing power, allowing for complex systems to be studied computationally for a time span of many nanoseconds. A prerequisite for the successful implementation of MD simulations is the detailed and accurate description of the intra- and intermolecular interactions. For this reason, a large number of force fields, both for H$_2$O and CO$_2$, have been reported in the literature during the last decades.

Our group takes advantage of recent developments of efficiently parallelized codes that allow significant reduction of computer time compared to serial executions and for this reason we use highly optimized open-source codes such as LAMMPS and GROMACS.

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