Molecular Simulation of the Structure and Diffusion of Carbon Dioxide in Salt Water: Implications for Carbon Storage

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Technologies for carbon capture are likely to have an increasing role in the abatement of global warming or climate change. Currently, the main focus of such technologies has been on land-based systems, most notably geo-sequestration. Ocean-based storage is a possible alternative to land-based technologies. The ocean's capacity to dissolve carbon dioxide is well known but the long-term storage capacity remains unknown. In particularly, reliable data is required for the high-pressure properties of carbon dioxide in seawater. Such data are almost impossible to obtain in situ and the high pressures and corrosive nature of the system create many difficulties for laboratory-based measurements. The system is also challenging for conventional theoretical approaches. For example, the traditional approach of developing equations of state has been of limited success for water. Accurate reference equations for pure water have been developed, which cannot be easily extended to mixtures. Conclusions reached from equation of state calculations are generally of limited value because of uncertainties in the theoretical representation of the underlying model and the need to fit equation of state parameters to experimental data. When used properly, molecular simulation is a useful alternative to the conventional theoretical approach. It allows us to investigate systems that are experimentally inaccessible with a greater degree of reliability than conventional theory. In this work, we report molecular simulation data at high pressures and different temperatures for the structural properties and diffusion of carbon dioxide in salt water. The system reflects the salient features of the deep ocean, allowing us to draw conclusions for carbon storage