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## ABSTRACT:

### Reactive CO<sub>2</sub> Diffusion in Aqueous Systems under Reservoir Conditions

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Developing predictive modeling of geological carbon storage for long term assessment requires the incorporation of diffusivity. The diffusion process of CO<sub>2</sub> in the latter systems can be described in three stages. First, the gas component in the CO<sub>2</sub>-rich phase moves toward the gas–liquid interface. Then, it crosses the interface to enter the liquid phase up to the solubility concentration. Finally, CO<sub>2</sub> diffuses into the liquid phase causing swelling and initiating reactions. Measurements of CO<sub>2</sub> diffusion coefficient in the liquid phase at reservoir conditions can be done either by (a) direct visualization of the concentration using X-Ray CAT scanning [1] or MRI techniques [2], or (b) indirect PVT approaches. The premise in adopting these techniques is that CO<sub>2</sub> does not react with the liquid phase. In an aqueous phase, however, CO<sub>2</sub> reacts with water to form HCO<sub>3</sub><sup>-</sup> and CO<sub>3</sub><sup>2-</sup> and with other ions to precipitate minerals such as calcite. The change in density profiles by CT images or gas mass balance in PVT cells cannot distinguish these different chemical forms of CO<sub>2</sub>. For assessments such as estimating total solution storage capacity, the latter point will not cause an issue as the total carbon is of interest. However, the diffusion coefficient as a parameter to feed reservoir simulators needs to be solely the aqueous phase CO<sub>2</sub> property since other chemical forms are considered separately. Here, by simulating reactive mass transport phenomena in liquid and porous medium coupled with thermodynamic calculations for the gas phase using moving mesh finite element method, we investigate the diffusion, swelling and reaction processes of CO<sub>2</sub> in a liquid phase. Based on the simulation results, CT based calculated diffusivities are modified for the kinetic behavior of CO<sub>2</sub>. Results indicate that the deviation in the calculated diffusion coefficient is more pronounced in alkaline condition with pH > 7.5. The simulation results are also consistent with the measured pressures and solubilities of CO<sub>2</sub> in the PVT cell at reservoir conditions.

[1] P. Babak and A. Kantzas, *Energy Fuels*, 33(8), 7009-7019 (1990).

[2] A. Fayazi and A. Kantzas, *Ind. Eng. Chem. Res.*, 58(23), 10031-10043 (1990).