Carbon dioxide in clay hydrates from classical molecular simulations

A. Botan[1], B. Rotenberg[2], V. Marry[2], P. Turq[2] and B. Noetinger[3]

[1] *Dep.t of Civ.and Env.Eng., MIT, Cambridge, Massachusetts, USA*
[2] *PECSA, CNRS and UPMC, Paris, France*
[3] *IFP-Energies Nouvelles, Rueil-Malmaison, France*

ABSTRACT: Underground storage of carbon dioxide (CO_2) in aquifers is one of the options for reducing the CO_2 emission to the atmosphere and the greenhouse effect. This assumes that CO_2 "disappears" as it is gradually absorbed by water. However, complete dissolution of CO_2 in water is a long-term process. At the beginning cap rock of aquifer plays role of a barrier to upwards CO_2 migration [1]. Clay-rich formation looks a suitable candidate for this purpose as a low permeability medium. The goal of this study is to understand how the presence of CO_2 can change the permeability capacity of clay. For this purpose, we consider the interaction between CO_2 and hydrated clays on the micro and nanoscale. We first investigated the thermodynamic properties related to swelling and the structure of CO_2 in hydrated Na-montmorillonite for micropores using the grand canonical Monte Carlo method [2]. The system is in equilibrium with a reservoir, which sets the chemical potentials of CO_2 and H_2O. We then used molecular dynamics to determine the diffusion coefficients for equilibrated configurations. The second part of this work is devoted to equilibrium thermodynamic and structural properties of the H_2O/CO_2 mixture in clay mesopores as a function of P/T conditions, pore size, chemical composition of clay.

1. B. Metz, O. Davidson, H. de Coninck, M. Loos, and L. Meyer (2005) *IPCC special report on carbon dioxide capture and storage*. Cambridge University Press, Cambridge
2. A. Botan, B. Rotenberg, V. Marry, P. Turq and B. Noetinger (2010) *Carbon Dioxide in Montmorillonite Clay Hydrates: Thermodynamics, Structure, and Transport from Molecular Simulation. J. Phys. Chem. C,* 114, pp 14962–14969