Considering gases in reactive-transport codes

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Geochemical and coupled reactive-transport codes, CHESS and HYTEC respectively, improved recently their representation of the gas phase, of its interaction with water, salts and rock and even of its mobility [1,2].

The integration of analytically solved cubic equations of sate (such as Peng-Robinson) and of their appropriate parameters, and of adapted flow/transport solvers allow to reproduce nicely laboratory measurements (fig.) as well as CO_2 storage field observation.

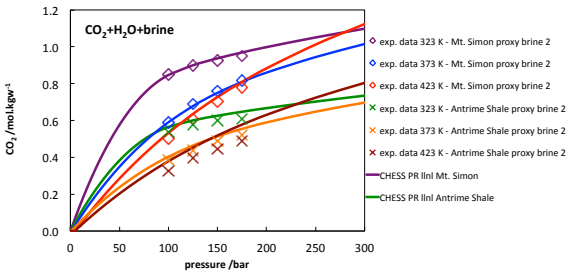

Figure Aqueous CO_2 molar fraction vs. pressure for CO_2 + H_2O + Mt Simon 1m NaCl + 0.2m $CaCl_2$ and Antrime Shale 3m NaCl + 0.7 $CaCl_2$ (symbols correspond to measurements [3], solid lines to CHESS simulations).

The obtained numerical results are very satisfactory when compared to both existing experimental data and numerical models. The relative simplicity of our approach (i.e. same EOS for each compound and limited parametrization) shall also be highlighted as it leads to comparable results.

CHESS/HYTEC are now able to handle non-ideal gas mixtures and then to simulate the injection/storage of high pressure complex gases into the undeground. They consequently offer important opportunities within various fields of applications such as CO_2 geological storage with impurities, or gas (CH_4, H_2…) storage in salt caverns.

[1] Corvisier (2013) *Mineral. Mag. Goldschmidt conference Florence (Italy)* **77**, 919. [2] Sin *et al.* (2017) *J. Chem. Eng. Data* **100**, 62-77. [3] Zhao *et al.* (2015) *Environ. Sci. Technol.* **49**, 1972-1980.