



## Characterization of CO<sub>2</sub> leakage into the freshwater body

Ashok Singh (1), Jens-Olaf Delfs (1), Habing Shao (1), Olaf Kolditz (1,2)

(1) Helmholtz Centre for Environmental Research - UFZ, Department of Environmental Informatics, Leipzig, Germany (ashok.singh@ufz.de, +49 341 235 1939), (2) Technical University of Dresden, Germany

Current research into Carbon dioxide Capture and Storage (CCS) is dominated by improving the CO<sub>2</sub> storage capacity. However, potential leakage of CO<sub>2</sub> can cause environmental problems, particularly if freshwater resources are nearby. In this regards, it is important to understand the chemistry of CO<sub>2</sub> and the water system. CO<sub>2</sub> leakage across the fluid interface (CO<sub>2</sub> and water) is controlled by the difference in the partial pressure of CO<sub>2</sub> in the storage and in the freshwater body. Once the CO<sub>2</sub> is in solution, it equilibrates with the bicarbonate and carbonate ions. According to Millero (1994) such a system can be characterized by two parameters out of the four: total alkalinity (TA), total carbonate (TCO<sub>2</sub>), fugacity of CO<sub>2</sub>(fCO<sub>2</sub>) and pH.

In the present modeling study, we are interested in the (i) CO<sub>2</sub> leakage into a freshwater body (while injecting CO<sub>2</sub> for storage) through an inclined fracture and (ii) characterization of the system by measuring fugacity of CO<sub>2</sub> and pH. According to work presented by Singh et al. (2012), about 31% of injected CO<sub>2</sub> leaks into the freshwater body. Solubility of CO<sub>2</sub> in water follows Henry's law, while the Henry constant, K<sub>0</sub> is calculated by an empirical relation developed by Murray and Riley (1971), which is a function of salinity and temperature. According to our results, pH and fugacity both appear to be a linear function of temperature.

To simulate the discussed problem, a corresponding numerical module has been developed for multi-component fluid flow coupled with heat and mass transport processes. Governing equations and Volume Translated Peng-Robinson equations of state are implemented within the object-oriented finite element code OpenGeoSys (Kolditz et al., 2012; [www.opengeosys.org](http://www.opengeosys.org)). Primary variables are pressure, temperature and salinity which are obtained by solving the governing equations in a monolithic way. The governing equations are discretized spatially within the context of a Galerkin approach, whereas the temporal discretization is performed using a generalized single step method.

### References:

Singh AK, Böttcher N, Görke U-J, Delfs J-O, Taron J, Kolditz O; A benchmark study on compositional fluid flow. *Energy Procedia*, 2012, (Accepted).

Millero FJ (1995) Thermodynamics of the carbon dioxide system in the oceans, *Geochimica et Cosmochimica Acta* 59: 661-677.

Murray CN, Riley JP (1971) The solubility of gas in distil water and sea water. *Deep-sea Res.* 18:533-541.

Kolditz O. et al. (2012) OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media. *Environ. Earth Sci.* 67, 589-599.