# *HT – Hydrogen Transfer* modeling with the *Nernst-Planck Solver* (*NPS*)

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We present a new framework for multiphase reactive transport simulations which couples electrochemical migration of aqueous ions, diffusion of gaseous species and thermodynamic equilibrium between solids, liquid and gaseous phase. We further apply this approach to the interpretation of *HT* experiment conducted at the *Mont-Terri rock laboratory* [1]. The *HT* experiment investigates the diffusion and reactions of gaseous $H_2$ in tight claystone, the *Opalinus Clay* (*OPA*). The *HT* setup supports gas injections and samplings from a drilled borehole perpendicular to the *OPA* bedding.

The newly developed *NPS* code considers coupling of the main processes already included in previous work [2]: (a) the diffusion of gases and solutes between borehole and *OPA* using the t*wo-film* model [3] adjusted for a porous media; (b) the diffusion of solutes inside *OPA* with the *Nernst-Planck* transport equation; and (c) microbial controlled reduction of $SO_4^{-2}$ by $H_2$ controlled with a *Michaelis-Menten* kinetic rate law.

*NPS* is a reactive transport code coupling the finite element framework *FEniCS* [5] and the chemical equilibrium solver *Reaktoro* [6]. *Reaktoro* is a Gibbs-Energy-Minimization based mass conservative solver which supports several EOS needed to model the multi-phase system in the borehole. *FEniCS* allows formulation of transport equations in a math-like straightforward syntax without the need to deal with underlying numerical algorithms. *NPS* can be easily altered to accommodate new source and sink terms or events and kinetic reactions that occur during the *HT* experiment.

We show that N*PS* achieves good agreement with the measured data using physically and chemically meaningful parameters. Thus, *NPS* serves as a flexible and easily usable tool for the investigation of chemically reactive environments.

[1] Vinsot *et al*. (2017) *Swiss J Geosci.* **110**, 375-390. [2] Appelo (2015) Technical note 2012-58 Mont Terri Project. [3] Liss & Slater (1974) *Nature* **247**, 181-184. [4] Appelo & Postma (2005) Geochemistry, groundwater and pollution 649p. [5] Alnaes *et al*. (2015) *Archive of Numerical Software* **3**. [6] Leal *et al.* (2016) *Adv. Water Resour*. **96**, 405-422.