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Modelling and Simulation of 4D GeoPET Measurements with COMSOL Multiphysics 4.2a

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Our GeoPET-method allows the 4D monitoring of (reactive) transport processes in geological material on laboratory scale (Gründig et al., 2007; Kulenkampff et al., 2008; Richter et al., 2005) by quantitative imaging of tracer concentrations. Recently we have conducted a long-term $^{22}Na^{+}$ in-diffusion experiment in an Opalinus clay drill core over a period of 7 months. We modelled this experiment with COMSOL Multiphysics ® 4.2a (3D convection-diffusion equation, PDE mode, PARDISO solver) for reproducing the observed spatiotemporal concentration distribution data with the following underlying equation for this anisotropic diffusion and adsorption:

$$\varepsilon \frac{\partial c_i}{\partial t} = \nabla (D_e \cdot \nabla c_i) - \rho \frac{\partial q}{\partial t}$$

— ε [-] porosity, c_i[mol/m^3] $^{22}Na^{+}$concentration, D_e [m^2/s] tensor of the effective diffusion constant for $^{22}Na^{+}$ in Opalinus clay, ρ [kg/m^3] bulk density and $\partial q/\partial t$ sink term for considering the sorption. By importing GeoPET images from various time steps and applying the Optimization Module (least square fit applying the Levenberg-Marquardt algorithm) to these images we efficiently determined best fit values e.g. of the diffusion tensor. Combined with the parameter sweep operation the sensitivity analysis is performed in parallel and covers the range of literature values for porosity and K_d values for $^{22}Na^{+}$sorption on Opalinus clay.

The experimental data could be reproduced quite well, but the obtained parameter values for diffusion parallel and normal to the bedding are slightly larger than reported in Gimmi and Kosakowski (2011). This is coherent with our observations of an emerging gas bubble in the central borehole tracer reservoir: Soil moisture tension in the partly unsaturated clay must have significantly influenced the transport regime by an additional advective component.

We suggest COMSOL Multiphysics ® is a powerful tool for the inverse modelling of timedependent, multidimensional experimental data as obtained by GeoPET.

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