

# Parameter Estimation of Anisotropic Diffusion in Clay with COMSOL Multiphysics®

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## Abstract

Our GeoPET camera is explicitly dedicated for and well capable of 4D monitoring of solute transport in dense geological material,  $c = c(x,y,z,t)$  [1-4]. We apply COMSOL Multiphysics® for reproducing our experiments and extracting parameter sets for our 4D problems [5-6]. By aligning simulated results of anisotropic diffusion in clay to our observations we are able to clearly differentiate and evaluate likely explicit sample features and transport processes.

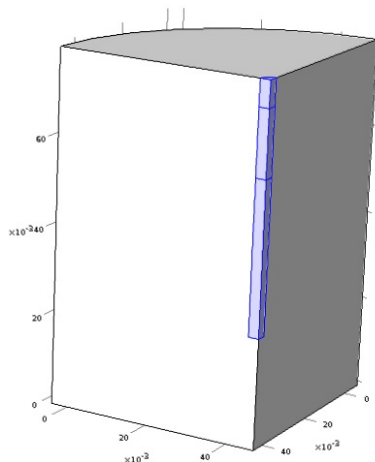
Use of COMSOL Multiphysics®: A quarter section of a cylinder (3D geometry, figure 1) is representing our clay core. The bedding of the clay is about vertical. A central bore allows for the application of a labelled pore water solution to diffuse into the material. Isotropic diffusion is assigned to the fluid in the bore hole, while anisotropic diffusion is assigned to the porous media (both with cdeg) (figure 2). From our non-invasive, spatio-temporal PET observations of the diffusion process in a real clay sample two 2D sets  $c_i(x,z)$  and  $c_i(y,z)$ , are extracted and provided to the Optimization Module for the parameter estimation for  $D_{xx}=D_{zz}$  and  $D_{yy}$ . A sensitivity analysis quantifies the effects on uncertainties regarding porosity  $n$ , initial concentration  $c_0$  and spatial resolution.

The 4D simulation results quantitatively nicely match with our 4D experimental results obtained in GeoPET experiments. In figure 3 a 2D image from with experimental data is superimposed by isolines from the simulation results.

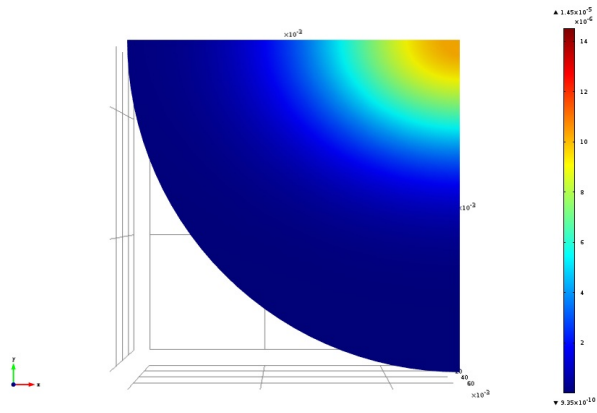
## Reference

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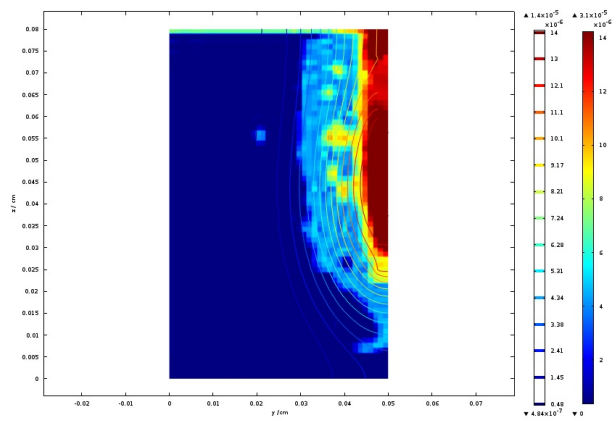
## Figures used in the abstract



**Figure 1:** Geometric features of clay drill core with central bore



**Figure 2:** Top view on simulated anisotropic diffusion, x-y-face



**Figure 3:** Superimposed isolines from simulation over measurement data, y-z-face