

Reactive transport modelling based on velocity fields obtained on drill core scale

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Extended Abstract

The objective of the EU project *BioMOre* is the development of new technological concepts for in situ recovering metals from deep European Kupferschiefer deposits using controlled stimulation of pre-existing fractures in combination with in-situ bioleaching. Considerable parts of the project are leaching experiments on lab scale and on small field scale at a selected location in an existing copper mine, as well as the related reactive transport modelling tasks including the required backcoupling from chemical reactions on the hydrodynamics as well as the upscaling. These tasks shall assist in the optimization of the bio-leaching efficiency, stimulating processes, as well as the environmental impact and sustainability assessment. Here we introduce our most recent technical advancement. It allows us to accomplish two tasks in one line of action: The extraction of effective hydrodynamic parameters in 3D for downstream modelling, and the upscaling from molecular process observations to reactive transport simulations on drill core scale.

For more than a decade a spatiotemporal visualization tool for transport process observations in dense material by means of PET (positron emission tomography) was developed [1-5]. Such quantitative GeoPET images are exceptionally sensitive to displacements of pico molar tracer quantities detected within 1 mm grids on laboratory/drill core scale. Now we reached a strategic milestone: A custom made image analysis algorithm is capable of quantitatively extracting velocity and porosity fields from such GeoPET image time series, even if the 4D image information includes discontinuous flow patterns (due to bottle neck effect related detection limits) and localized image artifacts. We present our approach with the aid of a) the data set with which the algorithm was validated, and b) provide an outlook for its application in the context of this EU project: the bio-leaching of Kupferschiefer.

From an observed fluid flow process in a dense core material by means of GeoPET (Fig. 1 left) the effective porosity and velocity field is extracted by our image analysis algorithm and this data is used in a forward numerical transport simulation and compared with the original fluid flow process (Fig. 1 right). Next steps will be the evaluation of non-reactive flow process observations in fractured calciferous sandstone from the Kupferschiefer ore deposit (Fig. 2), and the respective porosity and velocity field extraction for 3D reactive transport modelling in fracture and porous matrix by means of iCP [6] - an interface coupling the finite element based code COMSOL Multiphysics® with the geochemical code PhreeqC.

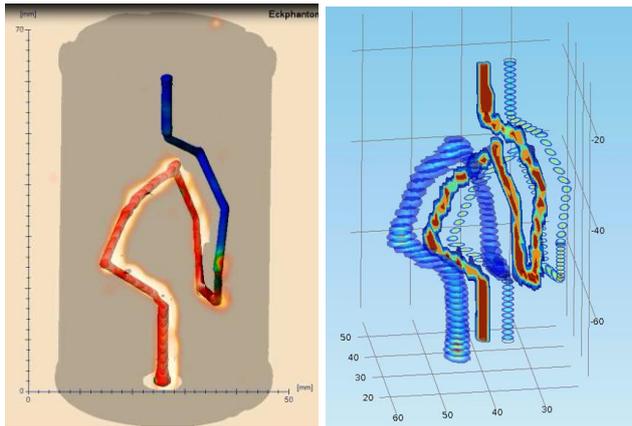


Fig. 1, left: Snapshot of a visualized fluid transport inside a tube embedded in a cement core by means of GeoPET; **right:** From right to left: extracted absolute value of $v(x,y,z)$ and extracted effective porosity $n(x,y,z)$; simulated $c(x,y,z,t)$ as obtained from a model with an unstructured grid. The observed and modelled transport processes agree well. The 3D velocity field extraction from experimental observations is therewith validated.

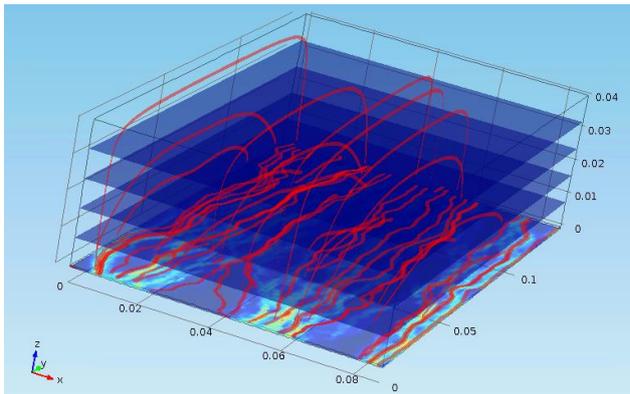


Fig. 2: Simulated velocity distribution (rainbow colour) and flow lines (red lines) inside a heterogeneous fracture (bottom) and adjacent porous calciferous sandstone (block above fracture): Outlook: Effective fracture velocities extracted from flow monitoring in fractured cores will be used in a 3D reactive transport model for estimating e.g. the effect of porosity/permeability change due to calcite dissolution and gypsum precipitation.

Key words: 4D image analysis, reactive transport modeling, in-situ leaching

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