FEFLOW piCHEM

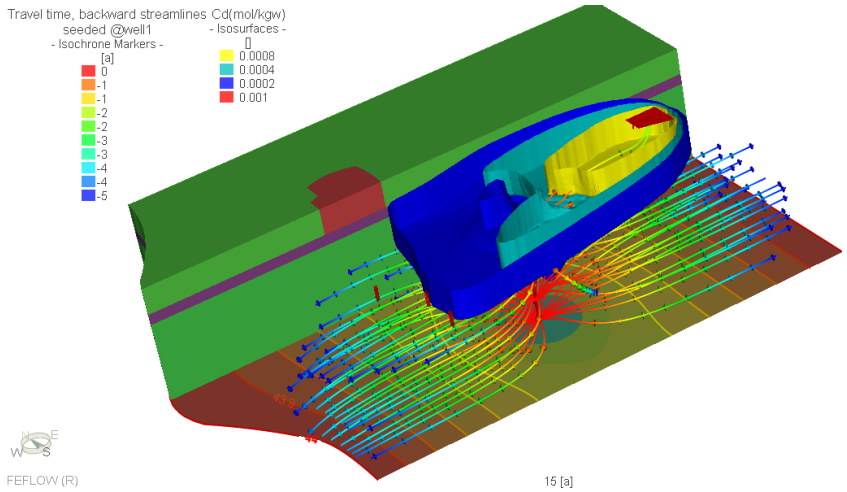
2D/3D geochemical modelling using PHREEQC in FEFLOW

Geochemical processes have a major influence on groundwater quality, for example in mining, for water supply and in groundwater-dependent ecosystems. Up to now, the simulation of these processes is often limited to batch reactions or transport along one-dimensional flow paths. Adapted software and improved computer hardware allow for much more nowadays!

piChem for FEFLOW has the power to drive this radical change. It supports the convenient extension of any two- or three-dimensional FEFLOW flow and transport model by geochemical reactions. With piChem relying on the PHREEQC reaction simulation engine (developed by the United States Geological Survey) and its standard definitions, the additional effort in model setup and results evaluation becomes manageable.

TYPICAL APPLICATIONS

- Simulation of contaminant fate
- Estimation of natural attenuation
- Planning of remediation measures
- Forecast of post-mining water quality (acid drainage)
- Leaching of radionuclides (low/high grade) and heavy metals from waste dumps
- Simulation of infiltration well clogging
- Solution mining
- Karst formation



Simulation of a heavy metal spill: 3D isosurfaces of Cadmium concentration and streamlines

BENEFITS

- Easy workflows through integration in FEFLOW
- Result visualisation in FEFLOW
- Relying on the state-of-the-art capabilities of PHREEQC
- 2D/3D flow and transport simulation
- Reaction definition by PHREEQC input scripts (in PHREEQC GUI or text editor)

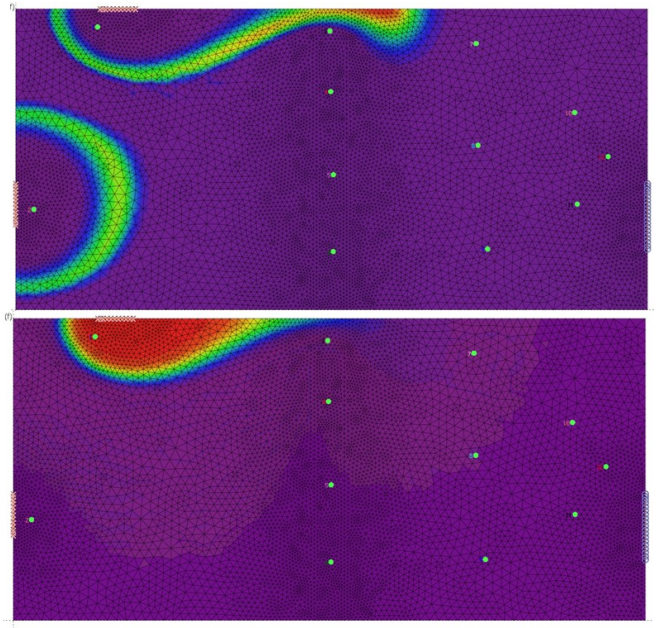
FEATURES

Ability to model:

- Activity corrected solution speciation
- Mineral dissolution/precipitation
- Solid solution reactions and ion exchange reactions
- Surface complexation reactions with optional diffuse double layer calculations
- Gas phase exchange reactions
- Temperature and pressure dependent reactions
- Advanced calculations of solution density from ion composition
- Kinetic reactions with possible dependency on solution speciation using PHREEQC's scripting capabilities and rate integrators

CATION EXCHANGE AND KINETIC DISSOLUTION

Complex reactions based on activity corrected solution speciation and the default PHREEQC database are used in this example following the MoMas benchmark (www.gdrmomas.org). It serves for demonstrating the capabilities of piChem in natural environments. The geochemical model combines the simulation of the snow-plough effect induced by cation exchange with the kinetic dissolution and precipitation of calcite according to the Plummer's complex rate expression.



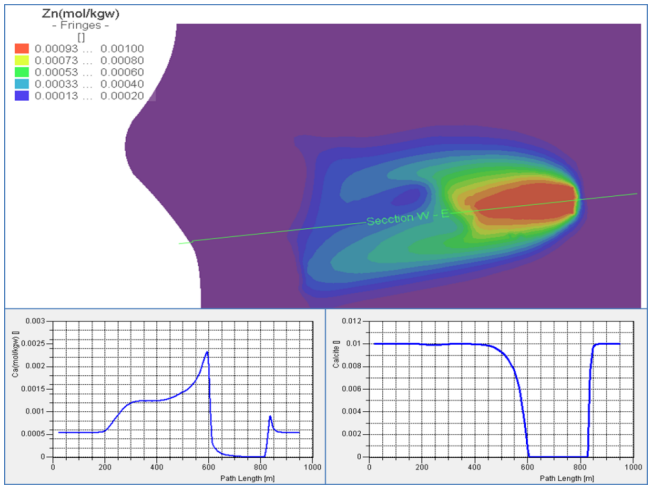
Calcite and Magnesium distribution at time 0.0001 days.

3D AQUIFER SIMULATION WITH HEAVY METAL SPILL AND SURFACE COMPLEXATION

piChem was used to represent the geochemistry of a heavy metal spill (Cd, Cu, Pb and Zn) with detailed ion speciation and retention due to surface adsorption.

The simulated processes are mineral dissolution/ precipitation, cation exchange and surface complexation with variably charged surfaces. The solution is in equilibrium with a calcite phase and the kinetic dissolution and precipitation of a large amount of quartz in the aquifer are considered.

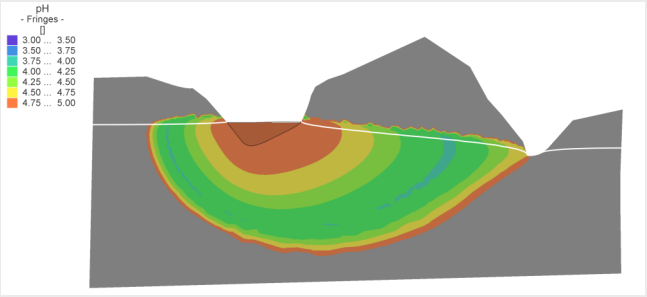
UNDERSTANDING ACID MINE DRAINAGE



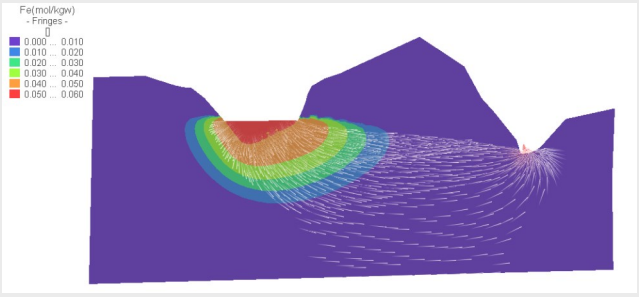
Distribution of a Zinc plume and concentration profiles of Calcium and Calcite.

Acid rock drainage naturally occurs within some environments as part of the rock weathering process, but is exacerbated by large-scale earth disturbances characteristic of mining and other large construction activities, usually involving sulfide minerals.

Typically the important physico-chemical processes takes place at the interface between saturated and unsaturated rock. While FEFLOW can easily simulate the complex 3D flow patterns due to infiltration, piChem can be added to deal with the In-situ chemical processes highly depending on pH.



Evolution of the pH distribution as a result of the reaction.



Distribution of the total iron concentration (Fe) infiltrated from a tailings facility and the Darcy velocity vectors.

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