Paleohydrogeological Reactive Transport Model of the Olkiluoto Site (Finland)

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Introduction

The safety assessment of the deep geological repository of Olkiluoto (Finland) requires the evaluation of the influence of the (past) progressive land uplift on groundwater dynamics and chemistry.

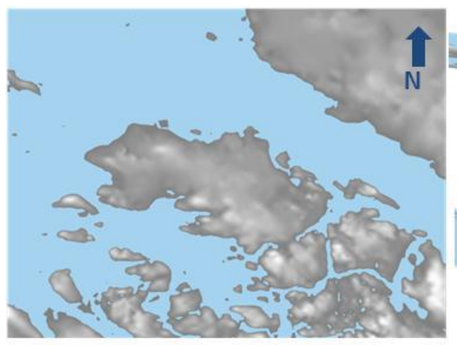
With this objective in mind, we have developed a three dimensional paleohydrological reactive transport (PRT) model of the Olkiluoto site. The model considers the most relevant deformation zones, which are represented as two-dimensional planes in a three-dimensional domain.

Abiotic and biotic reactive transport simulations have been carried out using the interface COMSOL-PHREEQC (iCP - Amphos 21). Abiotic simulations are focused on the evaluation of the mineral buffering capacity. Biotic simulations aim at getting insight into microbially mediate sulphate reduction processes.

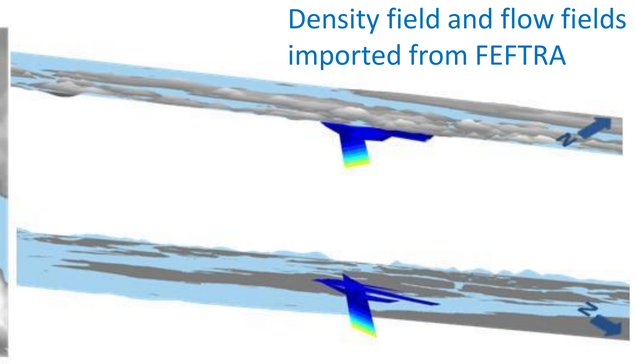
Numerical model

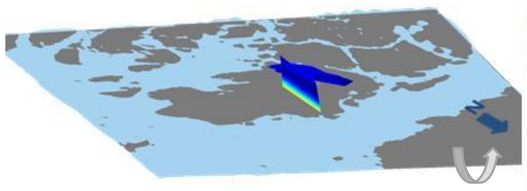
- Hydrogeological patterns are based on the geometry and results of an existing regional-scale model (i.e. FEFTRA model, Löfman & Karvonen, 2012).
- Heterogeneous geochemical initial conditions are defined based on the results of previous studies (POSIVA 2011-02).
- Different chemical reactions (e.g. equilibrium and kinetic mineral dissolution and precipitation, cation exchange, microbially mediated sulphate reduction) are accounted for.
- The simulations have been done using the interface Comsol-Phreeqc (iCP - Nardi et al., 2012).

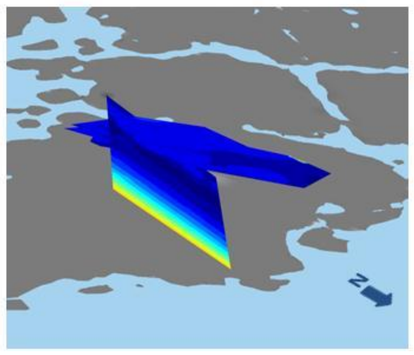
Model features

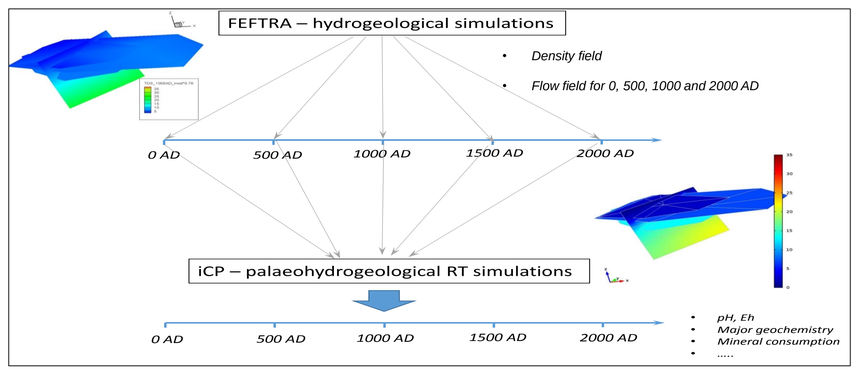


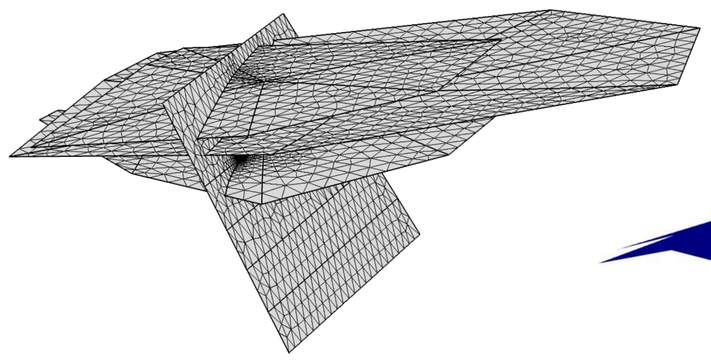
Density field and flow fields imported from FEFTRA

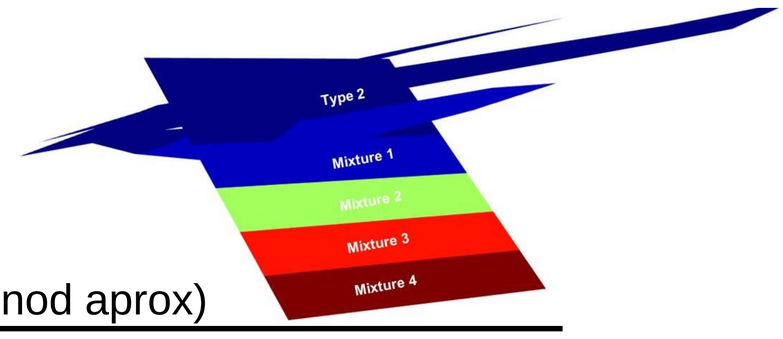












Chemical processes

(1) calcite and pyrite/FeS(am) dissolution/precipitation;
(2) aluminosilicates weathering; (3) cation exchange reactions;
(4) aqueous redox reactions

Bacterial growth rate (Dual Monod aprox)

$$r = q\,[X]\frac{[ED]}{[ED]+K_{ED}}\frac{[EA]}{[EA]+K_{EA}}$$

$$\frac{d[M]}{dt} = \gamma \cdot rate - D \cdot [X]$$

$$q = 1.39x10^{-6}\left(mol_{ED} \cdot mol_{bio}^{-1} \cdot s^{-1}\right.$$

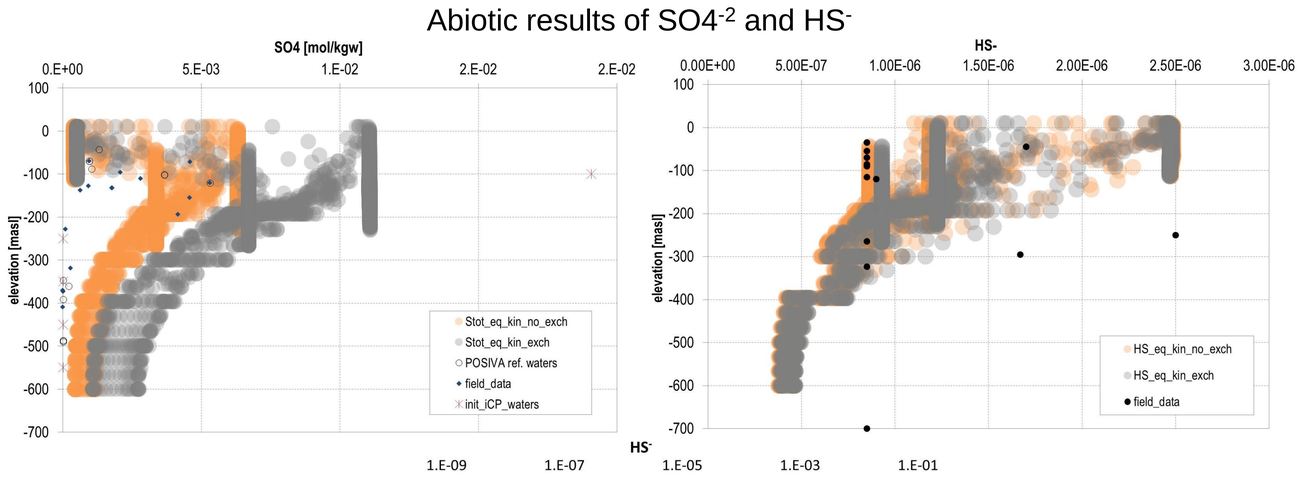
$$K_{ED} = K_{EA} = 9.00x10^{-4}(mol_{ED}/L$$

$$yield = 0.0261\ (mol_{bio}/mol_{ED})$$

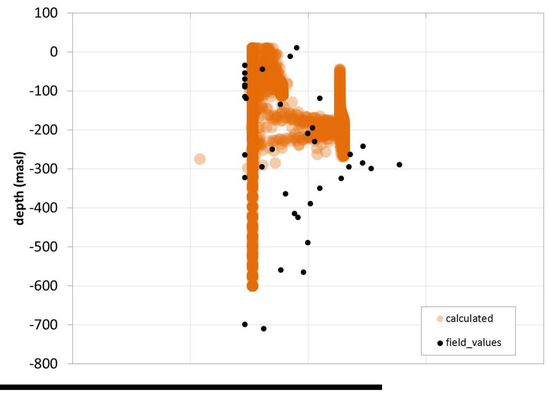
$$Decay = 5.79x10^{-8}(s^{-1})$$

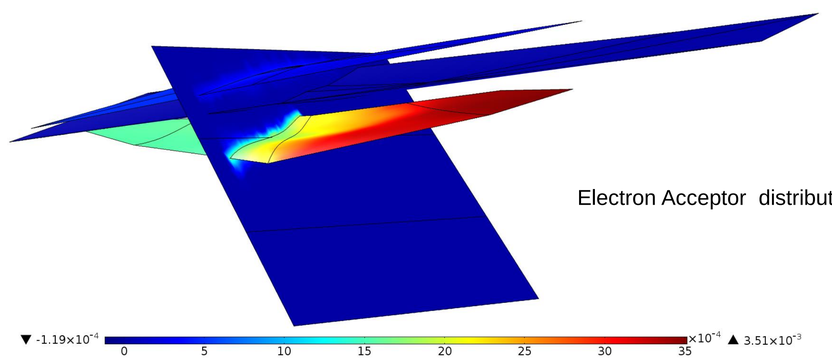
Results

Abiotic results of $SO4^{-2}$ and HS^-

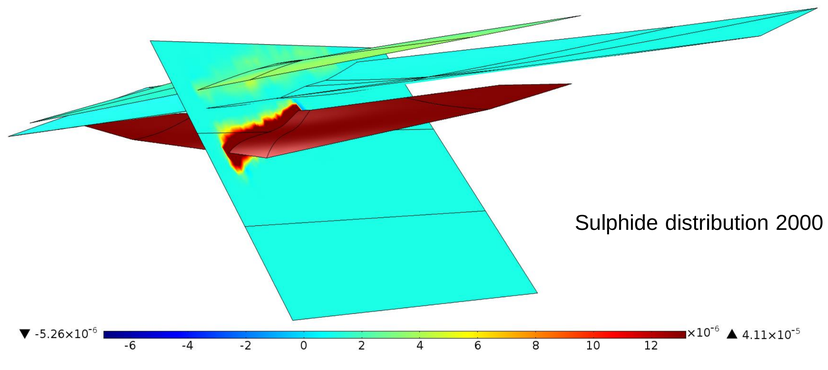


Biotic results of HS^-





Electron Acceptor distribution 2000 AD



Sulphide distribution 2000 AD

Conclusions

- A complex reactive transport model has been successfully implemented and solved with iCP. This complexity comes from geometrical features, geochemical reactions and flow conditions implementation from FEFTRA
- The reactive transport model accounts for the exchange of mass between the mobile domain (fractures) and the surrounding matrix blocks.
- The model results, which fit well with measured data at Olkiluoto, help to infer key information about the buffering capacity of the medium.
- The results of the biotic simulations fit well the sulphide field data (HS^-)

References

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