An equivalent K_d-based radionuclide transport model implemented in Comsol

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Introduction

Radionuclide sorption is often simulated using a lumped approach where retention processes are represented by the distribution coefficient (K_d), which relates the radionuclide mass retained in the solid phase to its aqueous concentration. K_d-based simulations rely on two strong assumptions: K_d depends on soil properties and is constant in time. However, sorption processes depend also on the fluid characteristics, which can vary in space and time.

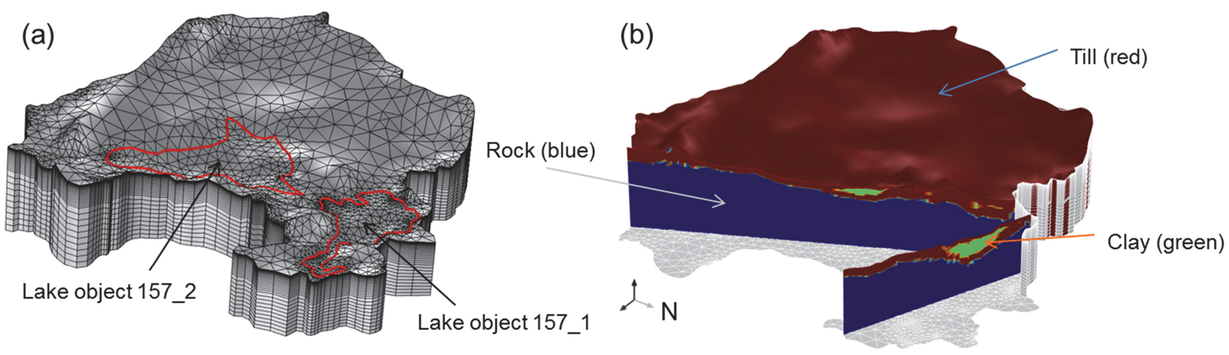

Figure 1. The near-surface system at Forsmark. (a) 3D mesh indicating the location of two discharge objects and the vertical discretization in the two blocks (vertical exaggeration x10z). (b) Geochemical model subdomains. The granitic rock (blue) is considered inert and the regolith is divided into till and clay domains.

Objective

The main objective of this work is to develop equivalent K_d-based radionuclides (RN) transport models that can reproduce the hydro-geochemical evolution of the soils at the site for spent nuclear fuel (Forsmark, Sweden).

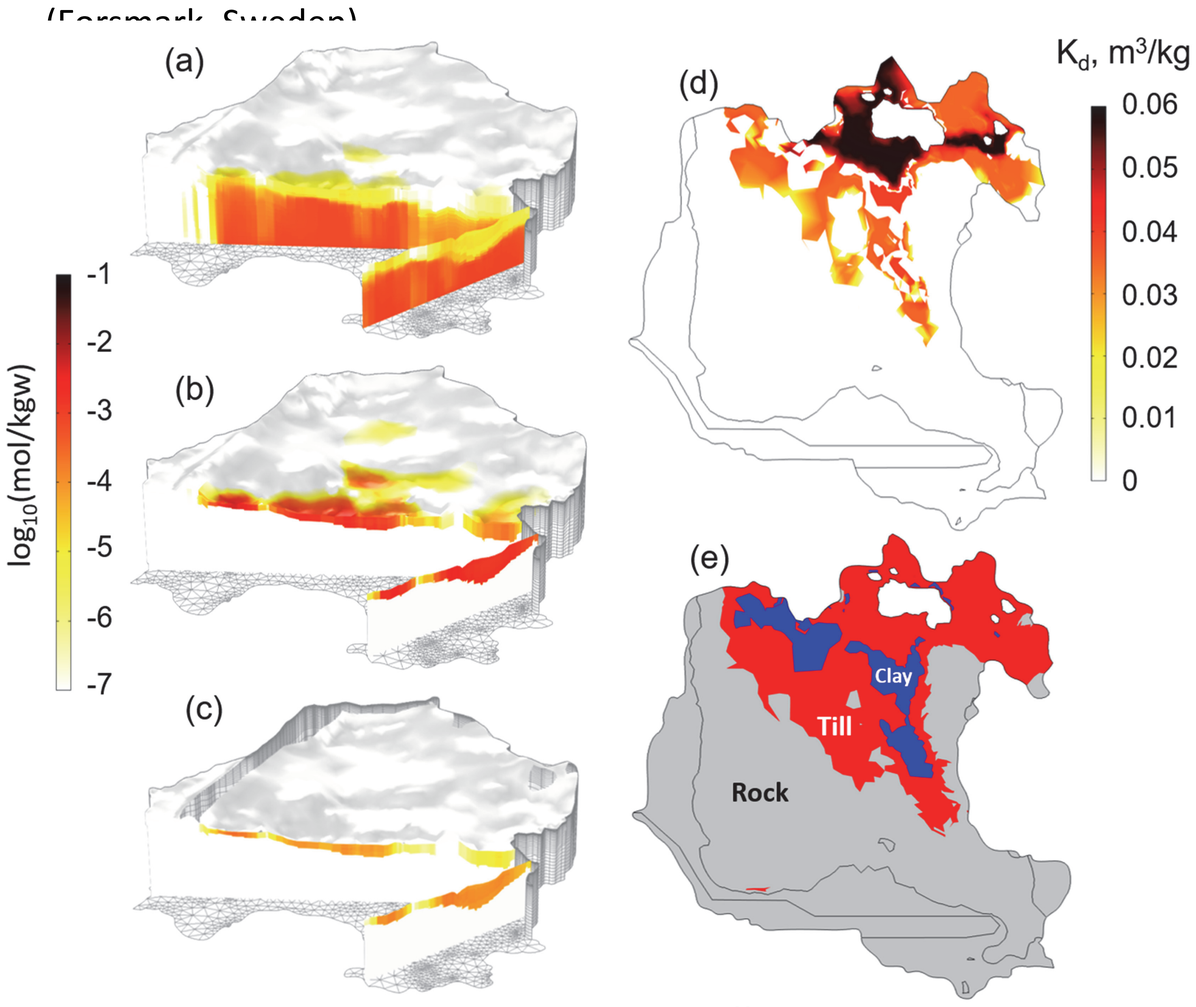

Figure 2. K_d interpretation methodology (retention of ^{90}Sr): 3D Distributions of (a) dissolved ^{90}Sr, (b) ^{90}Sr adsorbed on planar sites and (c) ^{90}Sr precipitated as strontianite are used to calculate the (d) equivalent K_d spatial field and the (e) dynamic 2-single K_d values.

Modeling approach

A 3D reactive transport model of the regolith was implemented in iCP (Nardi *et al.*, 2014). This model provides a K_d dataset that was used to build 2 equivalent 3D K_d-based models describing the retention of ^{90}Sr, ^{137}Cs, ^{235}U and Ra (Figure 2). The K_d models were implemented in Comsol using the Darcy's Law (Subsurface Flow module, Fluid Flow), and Solute Transport (Chemical Species Transport module) physics and accounts for steady state saturated-unsaturated flow assuming constant recharge and RN transport with linear sorption.

Results

Breakthrough curves show discrepancies between both equivalent K_d-based transport models and the fully reactive transport model. The ^{137}Cs evolution suggests that a dynamic 2-single K_d values approach is better than an equivalent K_d spatial field approach (Figure 3).

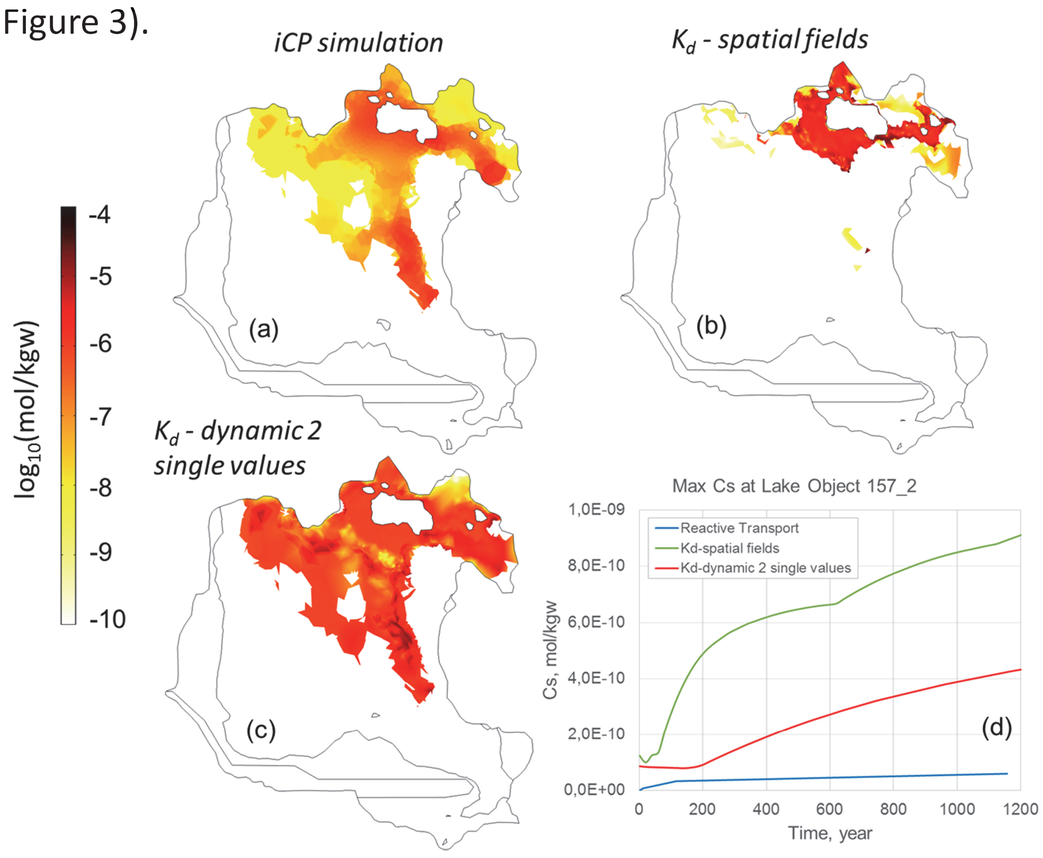

Figure 3. Concentration of retained ^{137}Cs (z = 3 m, after 1100 years) simulated with (a) iCP (fully reactive transport model) and Comsol: (b) equivalent K_d-spatial field approach and (c) equivalent dynamic 2-single K_d values. (d) Evolution of the maximum concentration of ^{137}Cs at the 157_1 lake object.

The formulation based on dynamic 2-single K_d values reproduces ^{90}Sr and ^{137}Cs retention better than the equivalent K_d spatial field approach (Figure 3), while this reproduces ^{235}U and Ra retention better than the former (Figure 4). This is because the dominant retention processes of ^{90}Sr and ^{137}Cs are mainly dynamic, while the main mechanisms of ^{235}U and Ra retention undergo local spatial variations that dominate over the temporal changes.

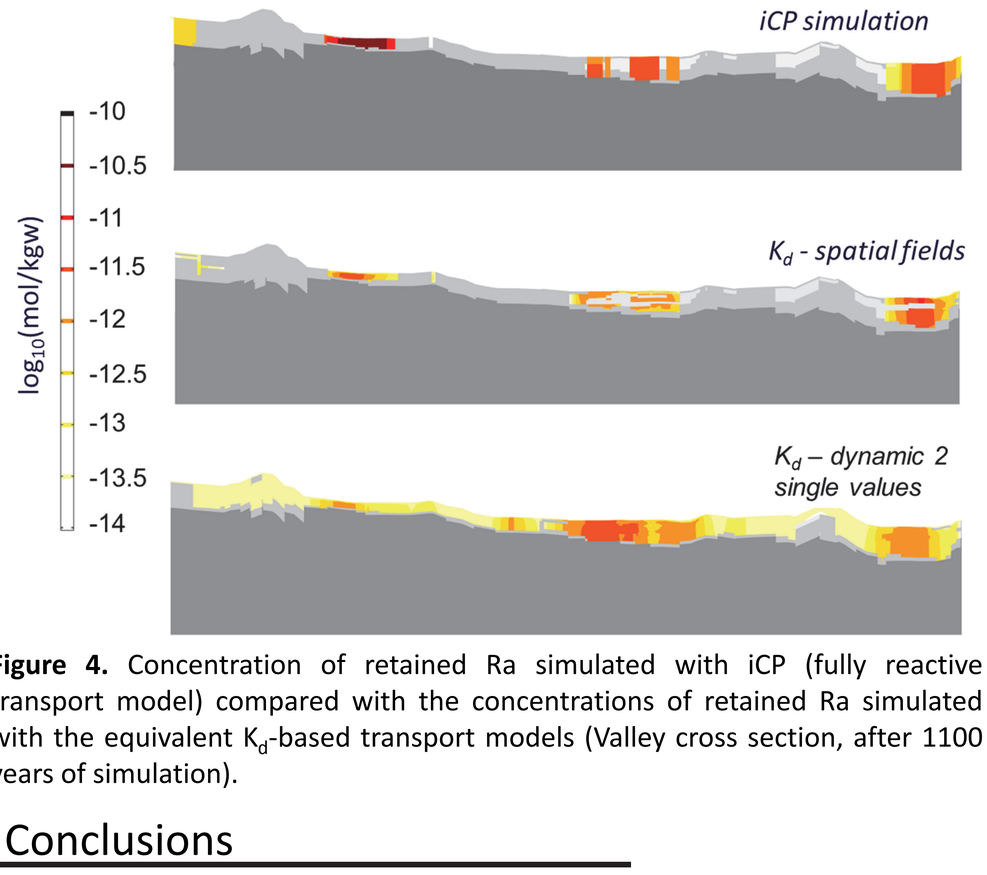

Figure 4. Concentration of retained Ra simulated with iCP (fully reactive transport model) compared with the concentrations of retained Ra simulated with the equivalent K_d-based transport models (Valley cross section, after 1100 years of simulation).

Conclusions

The equivalent K_d-transport models presented in this work may capture a big portion of the regolith evolution if the main processes governing its chemical behavior are interpreted properly. These models could be improved by approaches accounting for a dynamic update of the K_d values or by other alternative non-local in time and space approximations.

References

Nardi, A., Idiart, A., Trinchero, P., de Vries, L. M. and Molinero, J., 2014. Interface Comsol-PHREEQC (iCP), an efficient numerical framework for the solution of coupled multiphysics and geochemistry, *Computers & Geosciences 69*, 10-21 doi:10.1016/j.cageo.2014.04.011.

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