Quantification of porosity changes due to precipitation of cement materials with iCP

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Introduction

The Japan Atomic Energy Agency (JAEA) is being carried out an URL (Underground Research Laboratory) project in Mizunami city, central Japan. The project is a purpose-built generic URL project that is planned for a scientific study of the deep geological environment in fractured crystalline rock as a basis of research and development for geological disposal of nuclear wastes.

The concrete material using the URL construction is expected to be source of a hyperalkaline plume that can lead to porosity and permeability changes in the bedrock.

In this study, a 3D reactive transport model, developed with the interface COMSOL-PHREEQC (iCP) (Nardi *et al.*, 2014a), shows the evolution of the hyperalkaline plume and evaluates the influence of porosity changes on the rock permeability.

Model Set-up

The URL consists on two 500 m deep shafts and several galleries (Figure 1). Concrete lining at shafts and galleries, grout has been injected to minimize groundwater inflow volume.

iCP solves the reactive transport with a sequential non-iterative approach (SNIA). First the groundwater flow and conservative transport processes are modelled with heterogeneities and anisotropies in the hydraulic properties (hydraulic conductivity and porosity (Figure 2)). Then, the chemical reactions are modelled using PHREEQC (Parkhurst and Appelo, 2013) with the physical parameters provided in the first step. The groundwater flow modelling using COMSOL has been implemented with the Darcy's law physic while the modelling of transport process is implemented using a custom physic interface named Molal Solute Transport (Nardi *et al.*, 2014b).

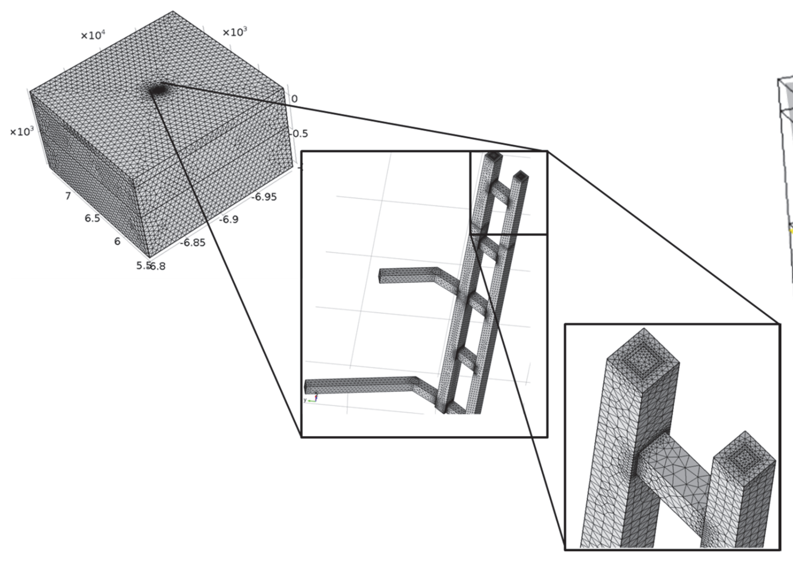


Figure 1. Detailed of the URL geometry and the refinement of the mesh.

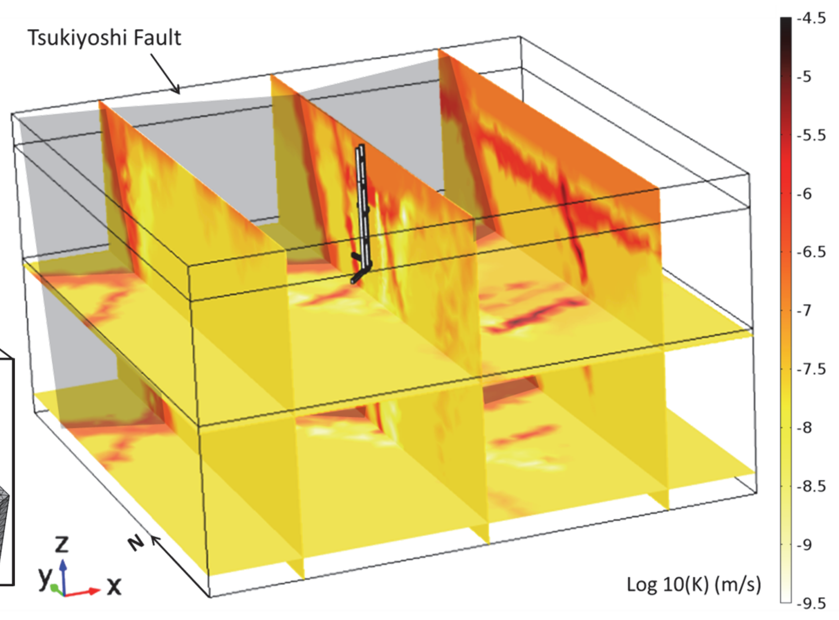


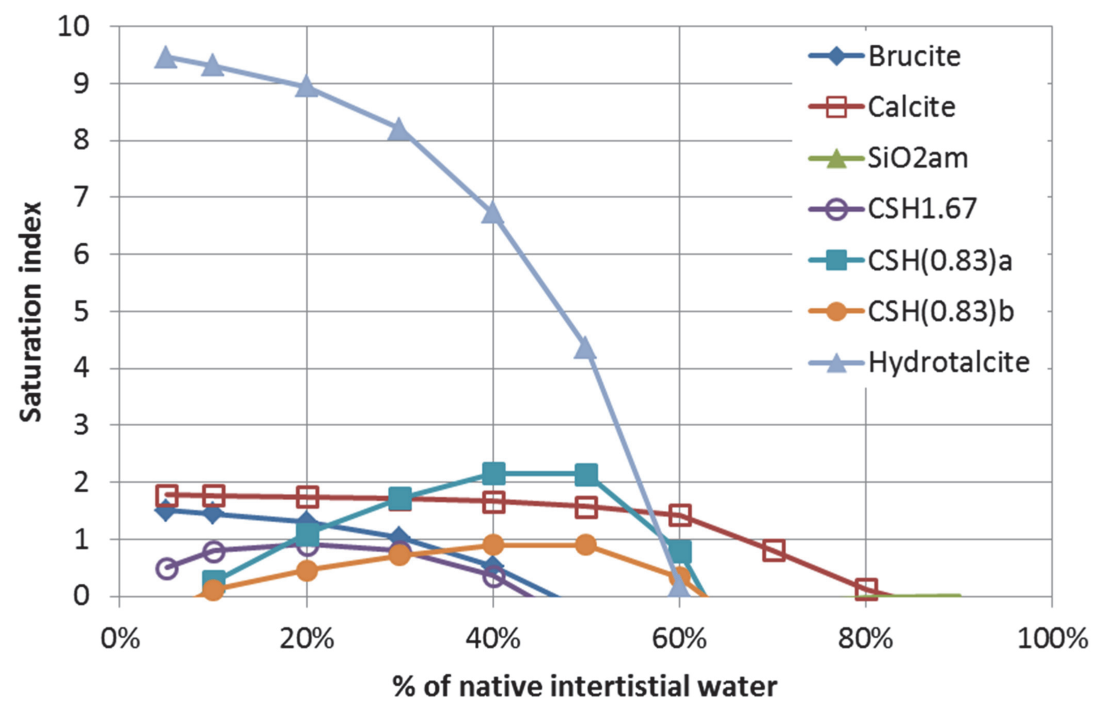
Figure 2. Rock hydraulic conductivity of the model domain with the URL located in the center of the domain .

Prescribed pressure and open boundary over the whole domain were assigned as boundary conditions for flow and transport respectively, with a total time simulation of 5000 years.

A preliminary 1D geochemical model of the interaction between the hyperalkaline concrete pore water and the native groundwater (Iwatsuki *et al.*, 2005) shows the oversaturation of different minerals phases (Figure 3). The precipitation of such minerals can lead to the variation of the porosity in the area. The relation between the permeability and the porosity have been implemented by the Kozeny-Carman equation (Costa, 2006):

$$k = C_{rk} \cdot \frac{\emptyset^3}{(1-\emptyset)^2}$$

Where k is permeability (m^2/d), C_{rk} is a material constant (m^2/d) and ϕ is the porosity (-).



Mineral notation	Reaction	Log_K*
Calcite	CaCO3= +1.000Ca+2-1.000H+ +1.000HCO3-	1.84897
Brucite	Mg(OH)2= +1.000Mg+2+2.000H2O -2.000H+	16.83953
Hydrotalcite_OH	Mg4Al2(OH)14:3H2O = 4Mg++ + 2Al(OH)4- + 6OH- + 3H2O	-56.0214
CSHjen	(CaO)1.666667(SiO2)(H2O)2.1 + 0.566667 H2O = 1.666667Ca++ + SiO(OH)3- + 2.333334OH-	-13.1659
CSH(0.83a)	CaO)2(SiO2)2.4(H2O)3.2 + 1.2 H2O = 2 Ca++ + 2.4 SiO(OH)3- + 1.6OH-	-19.1991
CSH(0.83b)	(CaO)0.83333(SiO2)(H2O)1.3333 + 0.50003H2O = 0.83333Ca++ + SiO(OH)3- + 0.66666OH-	-8.0014
Porlandite	Ca(OH)2 = +1.000Ca+2+2.000H2O-2.000H+	22.79937
SiO2	SiO2 + 1OH- + 1H2O = SiO(OH)3-	1.475988

*Based on CEMDATA07 version 07.02 (14.08.2008)

Figure 3. 1D model with mixing between grout material and natural groundwater. The image shows the saturation index of different mineral phases. The table shows the equilibrium constant for the different minerals phases involved in the model.

Model results

- In the simulated domain, high pH values (pH>11) extend less than 100 m downstream from the URL (Figure 4).
- The mixing between the plume and the native groundwater generates the precipitation of three minerals with a specific sequence (CSH(0.83), Hydrotalcite and Calcite).
- The precipitation of CSH and hydrotalcite occurs in the area where pH decreases from 12 to 10.
- Higher porosity changes are in relation with the precipitation of CSH and hydrotalcite. The maximum porosity change is about 9 % and leads to a permeability variation of about 45% for a simulation time of 5000 years.

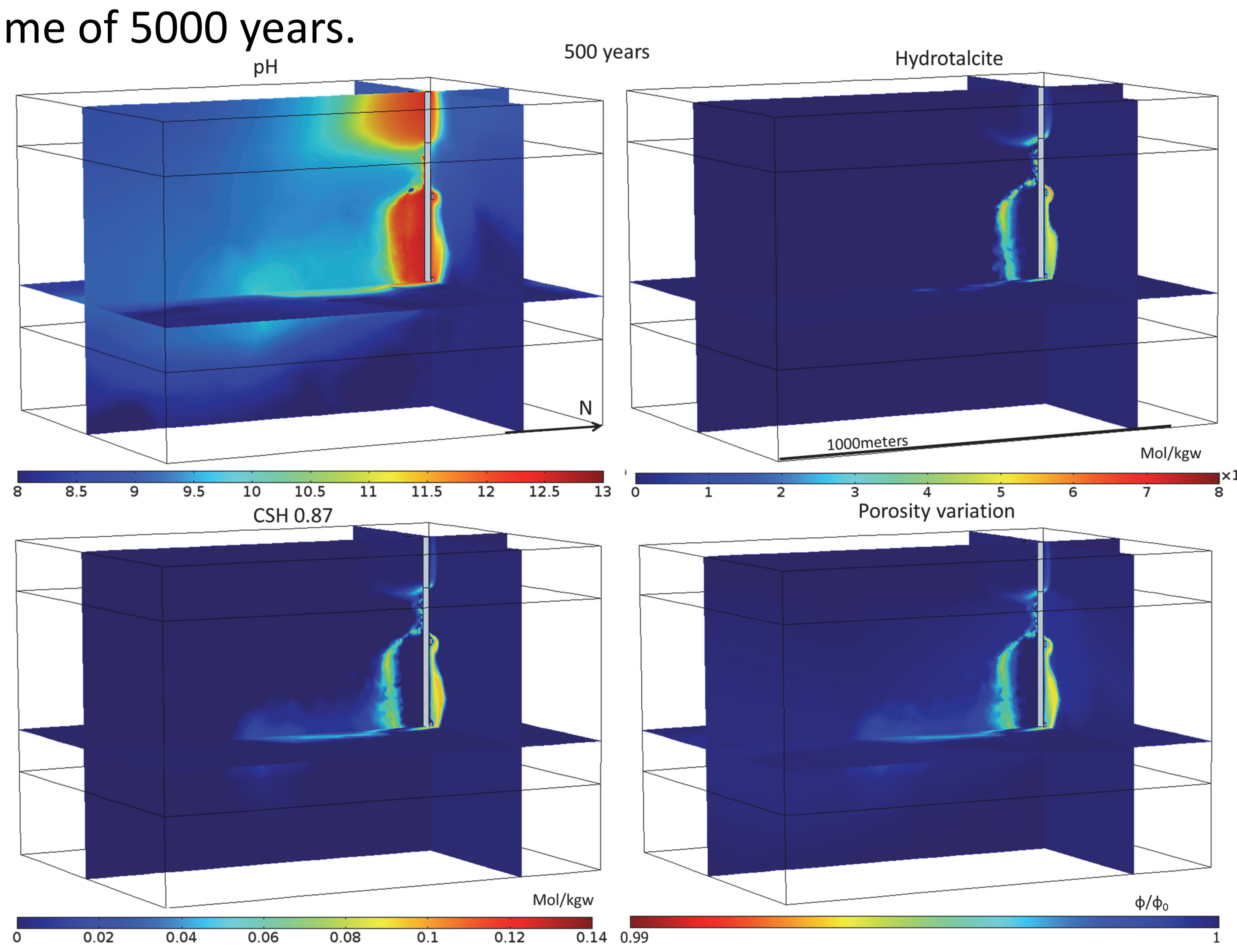


Figure 4. Groundwater pH ,different mineral precipitation and porosity variation for a simulation time of 500 years. Groundwater flows southwards.

Conclusions

- iCP is a flexible and powerful tool for quantitative integration of groundwater flow and geochemical models.
- iCP is able to model the geochemical processes in 3D large scale with long-term.

References

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