Long term evaluation on the groundwater chemistry due to cement materials with numerical simulation

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Introduction

The Japan Atomic Energy Agency (JAEA) is being carried out the Mizunami Underground Research Laboratory project in Mizunami city, central Japan. This laboratory is a purpose-built generic URL (Underground Research Laboratory) that is planned for a scientific study of the deep geological environment as a basis of research and development for geological disposal of high-level radioactive wastes. As part of the project, groundwater flow model has been developed using the commercial software ConnectFlow, which is capable to generate hydrogeological models but it cannot account for chemical processes. It is important to evaluate the effect of the cement materials present in the underground facility in the groundwater. Development of modelling method for understanding the temporal evolution of the concrete structures is a key process in the radioactive waste storage.

The objective of this study was to develop a reactive transport model that reproduces the evolution of the hyperalkaline plume in the bedrock, which is supposed to be generated by the concrete degradation. The precipitation of secondary minerals can reduce porosity up to the point to induce important changes on hydraulic conductivity.

Methods

The reactive transport model have been developed using iCP (interface COMSOL-PHREEQC)[1]. COMSOL[2] is a commercial software that solves a large range of different process, such as flow or conservative transport, using the finite element method. PHREEQC [3] is a well-known program which can be used as a speciation program to calculate saturation indices, the distribution of aqueous species, and the density and specific conductance of a specified solution composition.

The model developed is formed by the URL located in the middle of a “box” formed by granitic materials. The geometry and the spatial distribution of hydrogeological conditions (hydraulic conductivity and porosity fields) have been implemented in COMSOL from the ConnectFlow files (Figure 1 and Figure 2). The URL consists of two 500 m deep shafts and several galleries. In addition to concrete lining (blue area in the Figure 1), grout has been injected to minimize groundwater inflow volume. Grouted area matches with the volume in contact with concrete lining in this model (Figure 1).

iCP uses COMSOL[2] to solve the flow and the transport. The chemical part is solved by PHREEQC. The groundwater flow model has been implemented using the Darcy’s law physics and the transport process is implemented using a custom physics interface named as Molal Solute Transport.

The chemical composition of the grout is half of the portlandite and half of the CSH (1.67). This is a simplified composition taking into account the principal components involved in the alkalinity. The chemical composition of the groundwater has been obtained from Iwatsuki et al.[4]. Basically, this groundwater is in equilibrium with granites and has a pH of about 8.5.

A total time of 10,000 years of reactive transport simulations have been performed.

Results

Results of the model show that the high pH plume caused by dissolution of portlandite and CSH extends downstream. High values of pH (pH>11) extend less than 100 m downstream (Figure 3).

The mixing between the grout and the natural groundwater produces the precipitation of three minerals with a specific order. The first phases are CSH(0.83) and the hydrotalcite. The precipitation of hydrotalcite consumes most of the OH^- of the water and buffers the pH to about 10.5. The last mineral that precipitates is calcite, covering a larger extension in the rock and buffering the pH up to natural values.

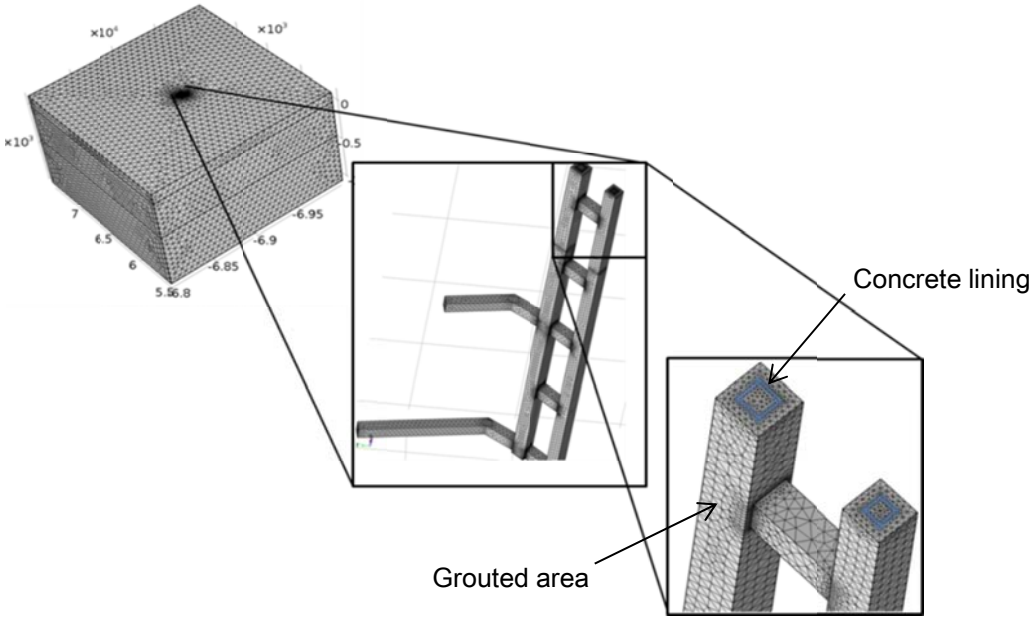

Figure 1: Detail of the URL geometry and the mesh employed in the groundwater flow model. The domain size is (2000x2000x1150 meters) and it is formed by 1,134,449 tetrahedral elements.

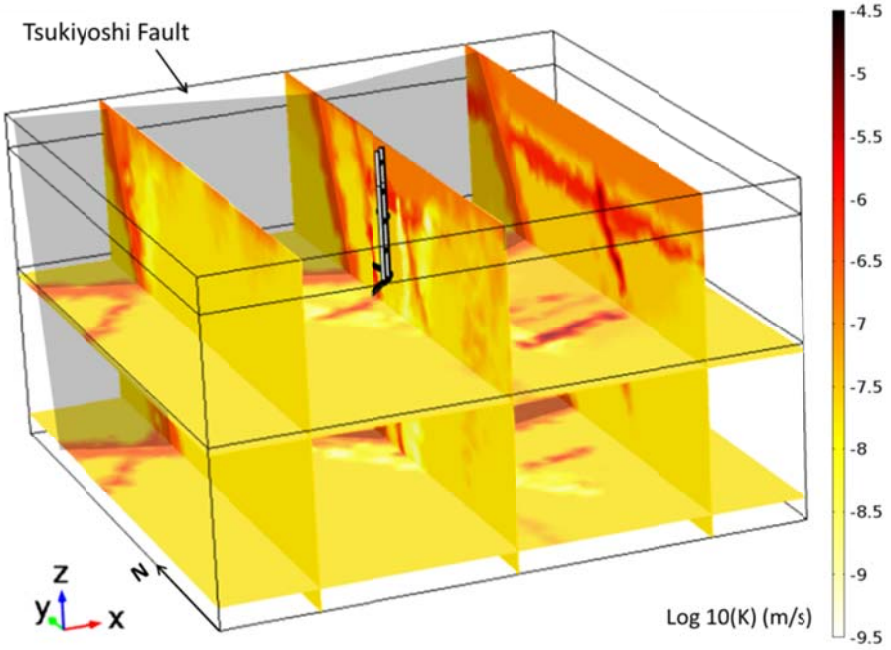

Figure 2: Hydraulic conductivity field of the rock domain implemented in COMSOL.

Discussion

Portlandite degradation is higher in the laboratory zone located upstream (northern border) and in areas where the water pore velocity is higher. The highest portlandite degradation rates are located about 200 meters of depth below the sedimentary rocks.

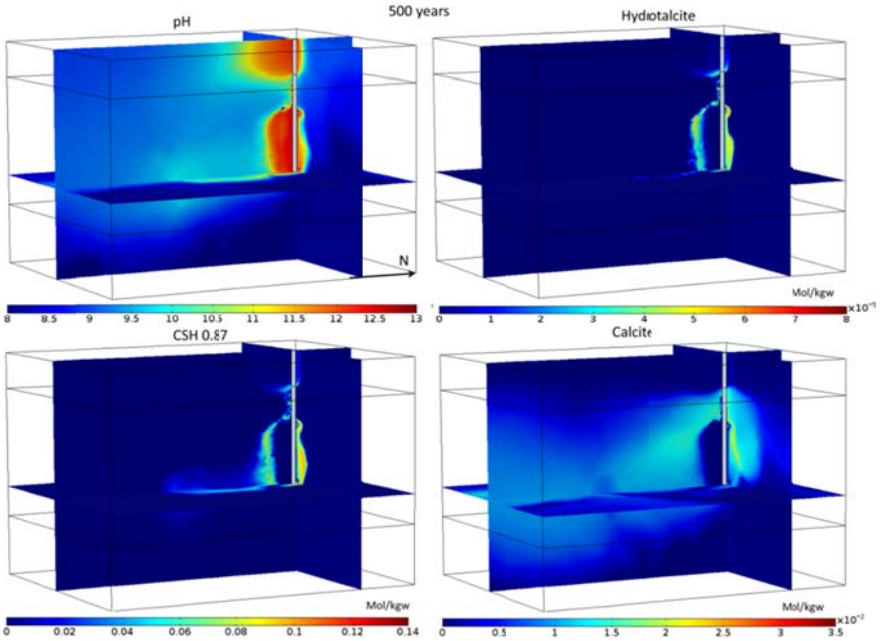

Figure 3: Groundwater pH and different mineral precipitation for a simulation time of 500 years. Groundwater flows southwards.

The high pH plume caused by dissolution of portlandite and CSH extends towards the downstream direction, but its extension is limited and buffered. High values of pH (pH > 11) extend less than 100 meters downstream. The high extension of the pH values > 11 are located in two areas characterized by low values of pore velocities. In these two areas, the mixing between the "grout water" and the native water is smaller, as a result produce less dilution.

The mixing between the grout water and the native groundwater produces precipitation of following three main minerals (CSH(0.83); hydrotalcite and calcite), occupying a larger extension and buffering the pH to almost the natural initial values.

The hydraulic shadow area located downstream the laboratory, which presents pH higher than 11, not present precipitation of mineral phases. The same effect is also observed for the sedimentary rock domain.

This study shows that iCP is a flexible and powerful tool for quantitative integration of hydrogeology and geochemistry. iCP allows to incorporate geochemical processes in 3D large scale COMSOL models and for long-time simulations.

References and Citations

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