Modeling of radionuclide transport in the overburden of a flooded salt mine

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ABSTRACT: At the last FEFLOW conference in 2012, we presented a groundwater flow and brine transport model of about 2 million elements to simulate the spreading of brine expelled from a flooded salt mine in the caprock and overburden (Poppei et al., 2012). The complex model is characterized by the existence of hydrogeologic units with strongly varying permeability as well as the effects of mineralization on fluid density and viscosity.

We extended this model to simulate the complex transport of radionuclides, including radioactive decay in chains and element and rock specific sorption. For safety assessments of the radioactive waste repository, it is the long-term radiation exposure in the biosphere that is of particular importance. Investigation of the possible environmental impacts of radioactive waste requires the identification of potentially dominating pathways of radionuclide transport from the repository to the biosphere.

We focus here in the experience gained from the numerical implementation of complex transport processes in this challenging model with non-linear fluid processes.

INTRODUCTION

An abandoned salt mine serving as a disposal facility for radioactive waste may be naturally flooded in the long term. In such a scenario, due to convergence of the mine openings, a highly saline brine contaminated with radionuclides will be expelled from the flooded mine into the surrounding rocks. This expelled brine will propagate through the caprock and the overburden and will become diluted before it reaches the shallow groundwater aquifers. At the same time, transported radionuclides will sorb and decay.

To simulate the propagation of the expelled brine and the transport of radionuclides, a 3D process model has been developed which considers the hydrogeological conditions and transport processes in order to calculate the flowpaths of the expelled brine and simulate the transport of radionuclides.

MODEL CONCEPT

Geometry and discretization

A vertical cross section with a length of 9 km is the basis for the FEFLOW 3D flow and transport model. This geologically representative 2D cross section is translated along the valley cut over a distance of 1000 m (Figure 1).
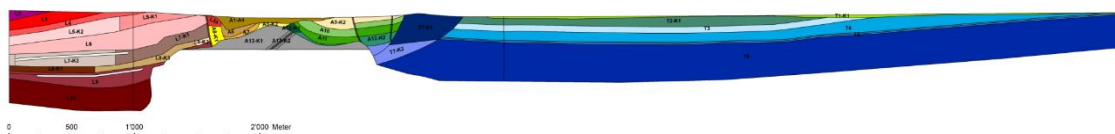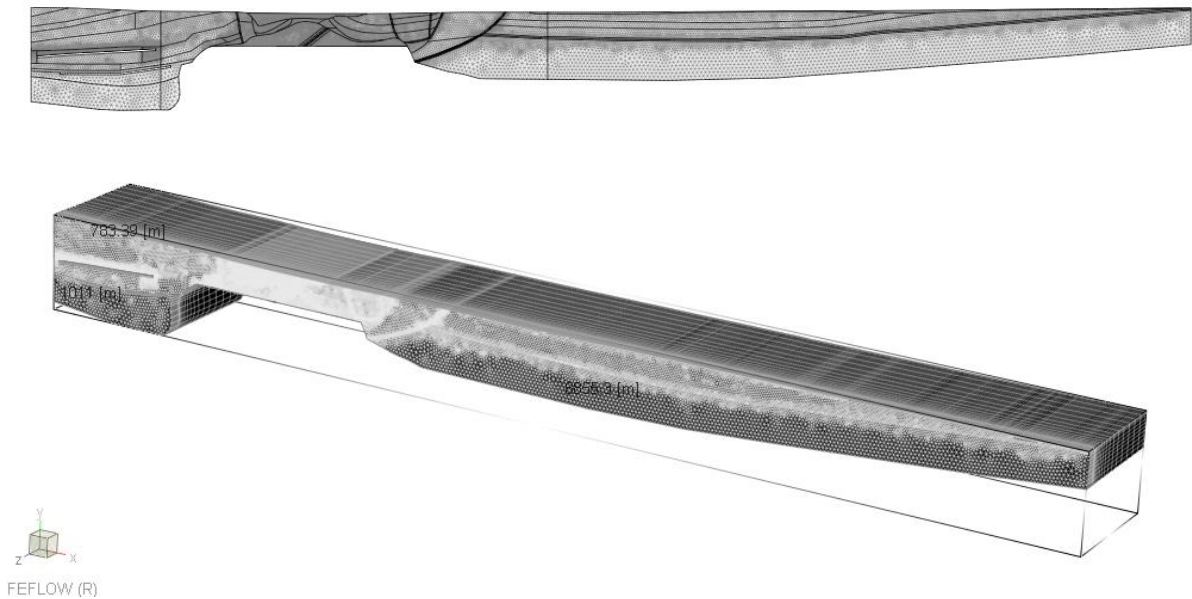
Figure 1: Model geometry and discretization

The model basis is the surface of the salt structure which contains the mine. It is assumed that the brine will be expelled into the model domain at a small area within the intersection of the surface of the salt structure and a highly conductive 2D structure within the caprock. The discretization of the vertical 2D cross section takes into account 15 different hydrogeologic units and has cell sizes between approximately 0.5 m in the vicinity of the highly conductive structure and 50 m in remote areas. The cross section is copied into 31 slices in the 3rd dimension with distances between slices gradually increasing from 10 m to 100 m. In total the model consists of roughly 2 mio. finite elements (Figure 1).

Parameterization

Constant parameter values are assigned within each hydrogeologic unit. Flow parameters include hydraulic conductivity and specific storage. Transport parameters consist of porosity, diffusivity, dispersivity, and the sorption and reaction coefficients. Note that both coefficients not only vary in function of the unit but in function of transported species as well. The amount of parameters is large and there are high property contrasts as can be seen on Figure 2 representing the conductivity distribution.
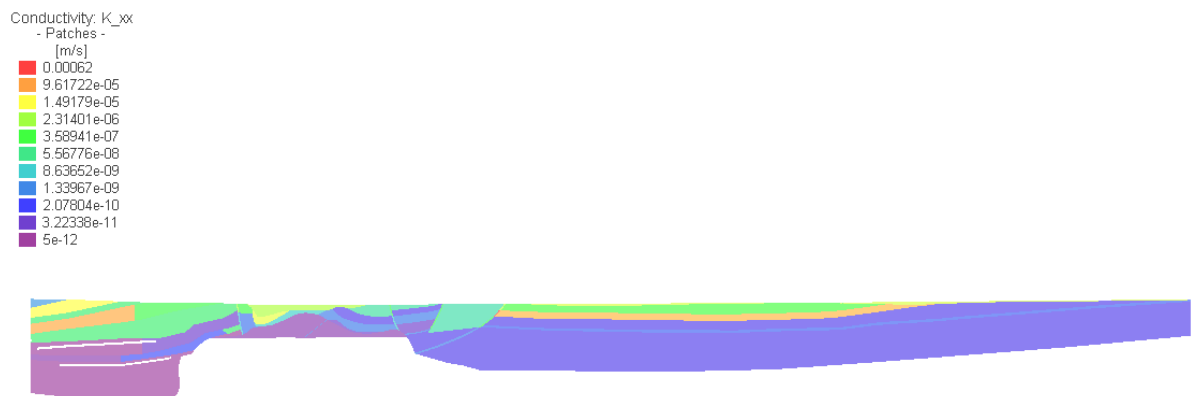

Figure 2: Conductivity distribution

Boundary conditions

Concerning boundary conditions for flow, a constant head boundary is set at the top, no flow boundaries at the bottom and sides and a time varying nodal injection rate above the repository. Concerning the transport of NaCl, a constant concentration corresponding to saturation is set at the contact with the salt structure and salt lenses and a concentration gradient of zero at sides. Finally a time-dependent concentration is set at the injection nodes for the radionuclide species.

Transport species

The model includes a total of 13 species that can be divided into two groups: the non-sorbing and the sorbing species.
The non-sorbing species including NaCl plus 3 "ideal tracers" used to simulate the transport of non-sorbing radionuclides (^{14}C, [36]Cl, [93]Mo, [126]Sn and [129]I). In order to simplify the simulation of the non-sorbing radionuclides, their decay is calculated through post-processing of the simulation results.
The sorbing species include 2 individual radionuclides ([94]Nb and ^{99}Tc) and 2 radionuclide chains:

- ^{238}U -> ^{234}U -> ^{230}Th -> ^{226}Ra
- ^{239}Pu -> ^{235}U -> ^{231}Pa

Sorption

Sorption is implemented with the FEFLOW Henry coefficient. The Henry coefficient is equal to the product of the solid rock density with the dissociation constant. It is function of both the geologic unit and the species considered.

$$\mathrm{K}_{\mathrm{d,FEFLOW}}^{\mathrm{i}} = \rho_{\mathrm{s}}^{\mathrm{m}} \cdot \mathrm{K}_{\mathrm{d}}^{\mathrm{i}}$$

Decay

The user-defined reaction equation is used instead of the degradation function implemented in FEFLOW due to the number of species (the degradation function is limited to models including a maximum of 9 species). It is used to implement the decay of individual radionuclides and chain decay.

$$R_1 = +k_1 \cdot \mathrm{Rate}_1 C_1^{n_1} + k_2 \cdot \mathrm{Rate}_2 C_2^{n_2} + \ldots$$

$$k_i = \begin{array}{ll} +1 & \text{creation} \\ -1 & \text{decomposition} \end{array}$$

The reaction rate is equal to the product of the decay rate (natural logarithm of 2 divided by the half-life) with the rock porosity and the retardation coefficient.

$$Rate_i^m = \frac{\ln(2)}{t_{1/2i}} \cdot \Phi_m \cdot R_i^m$$

Finally, the retardation coefficient is function of the rock porosity, the solid rock density and the dissociation constant.

$$R_i^m = 1 + \frac{1 - \Phi_m}{\Phi_m} \cdot \rho_s^m \cdot K_d^i$$

SELECTED RESULTS

Figure 3 shows the concentration of ^{99}Tc at about 60,000 years after the start of the injection of the contaminated brine. The highly conductive structure acts as a preferential pathway for the transport of ^{99}Tc. The sorption coefficient of ^{99}Tc in the highly conductive structure is relatively low. In contrast, Figure 4 shows the concentration of ^{238}U at about 100,000 years after the start of the injection. Because the sorption coefficient of ^{238}U in the highly conductive structure is high, the latter does not constitute a preferential pathway for the transport of ^{238}U. The sorption coefficient is assumed to be null in the caprock.
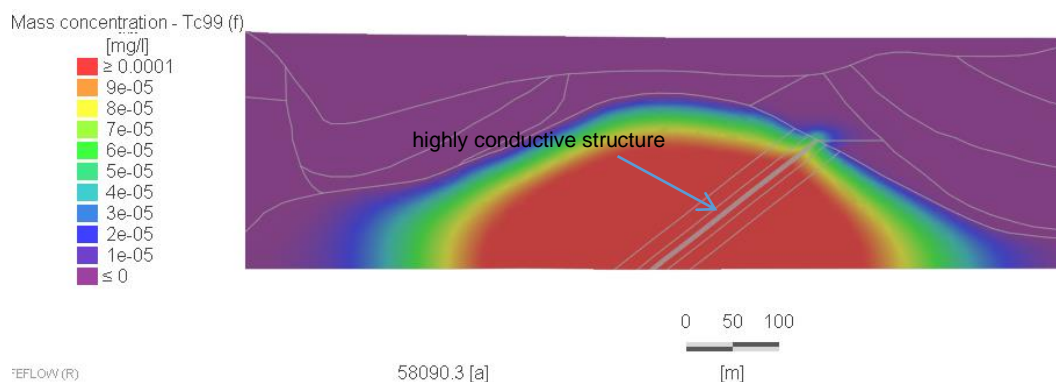
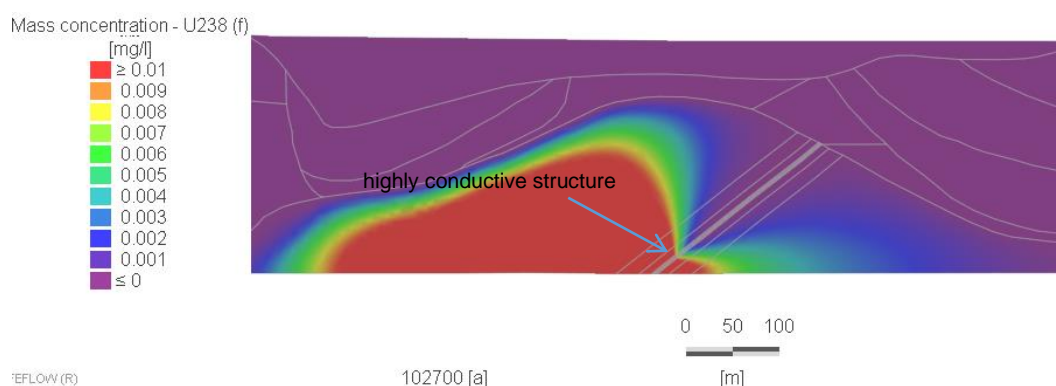**Figure 3: Distribution of ^{99}Tc at about 60,000 years (cross-section above the interface with the mine)**

Figure 4: Distribution of [238]U at about 100,000 years (cross-section above the interface with the mine)

CONCLUDING REMARK

The main challenge pertaining to the implementation of this complex flow and transport model was to find the adequate spatial and temporal discretization. It has been a lengthy trial and error process. The mesh has been globally and locally modified and the maximum time step length adapted several times in order to mitigate numerical oscillations and model crashes at every step of the model implementation. Furthermore numerical and solver parameters have been varied in order to find the most appropriate combination.

REFERENCES

Poppei, J.; Resele, G. & Wenderoth, F. (2012): 3D process modeling of groundwater flow and brine transport in the overburden of a flooded salt mine; International FEFLOW User Conference, September 3-7, 2012, Berlin, Germany

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