Numerical Simulations of Radionuclide Transport through Clay and Confining Units in a Geological Repository using COMSOL

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Abstract: The Swiss Federal Nucelar Safety Inspectorate (ENSI) conducts independent calculations of advective-diffusive transport of safety relevant radionuclides in order to review safety analyses done by the Swiss implementer Nagra (National Cooperative for the Disposal of Radioactive Waste). Two model case studies of generic geological repositories for radioactive low- and intermediate level (case A) and long-lived intermediate level waste (case B) are presented in this study. Case A includes the host rock ("Opalinus Clay") and confining units (claystone, marl and sandy limestone, Dogger), whereas case B considers the host rock and conservatively neglects the confining units. Among other codes, ENSI uses COMSOL ("Darcy's law" and "Solute Transport" modules) for radionuclide transport and resulting dose calculations.

Keywords: Radioactive waste, geological repository, safety assessment, radionuclide transport, dose calculation.

1. Introduction

The sectoral plan that defines the procedure and criteria for site selection of deep geological repositories for all categories of waste (high-level and low- and intermediate-level waste) in Switzerland started in 2008 and will last for about ten years. ENSI is in charge of reviewing the proposals and safety assessments for geological repositories submitted by the Swiss implementer Nagra. In order to review Nagra's safety analyses, ENSI performs independent calculations using COMSOL and other codes. Benchmark calculations have been conducted and the results of four different codes have been compared earlier (see Sentis et al., 2009). In this report selected results of calculations conducted for low- and intermediate-level waste repositories using COMSOL will be presented.

2. Conceptual Model

The presented model aims at calculating the radionuclide transport from a geological repository into the biosphere and to estimate the corresponding annual dose. The presented study focused on the radionuclides I-129, Se-79 and Cl-36, which show small retention in the different barrier systems of a geological repository. The present study considers two model cases:

Case A considers a repository for low and intermediate level waste inside the "Opalinus Clay" host rock and the confining units ("Brauner Dogger"). Case B represents a repository for long-lived intermediate level waste inside the "Opalinus Clay" host rock, where the confining units were conservatively neglected.

2.1 Geology at study area

Figure 1 shows a conceptual illustration of the cavern and several assumed model cases with corresponding transport path lengths.

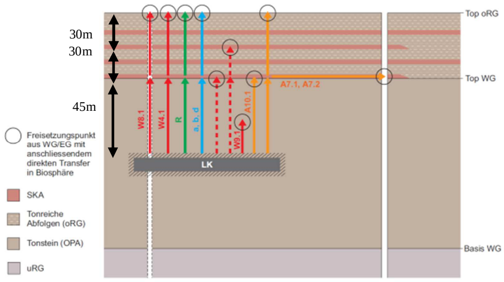

Figure 1: Longitudinal profile of the cavern, the host rock and some confining units (from NTB 10-01, Nagra, 2010, modified).

An excerpt of a geological profile of a potential siting region for a geological repository is shown in figure 2. The "Opalinus Clay" will be used as the host rock, confining units are considered in the model as well. The sediments of the "Brauner Dogger" can include layers of sandy limestones. These are implemented in the numerical model as a separate layer of homogenous porous medium.

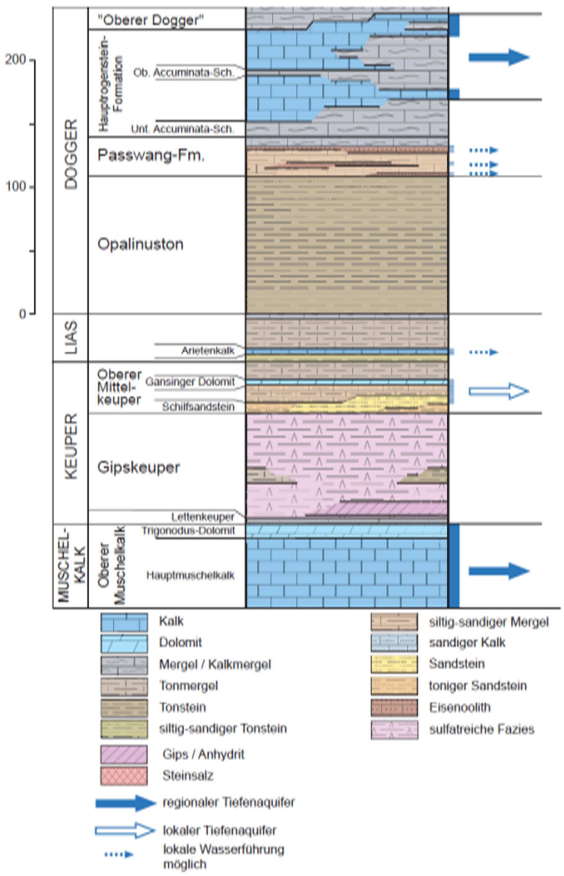

Figure 2: Excerpt of a stratigraphic profile of a potential siting region for a geological repository (from NTB 10-01, Nagra, 2010, modified).

2.2 Model geometry

The according model geometry based on the geological profile is represented by the gray area in figure 3. Neighboring caverns are indicated by the dashed lines. Horizontal distances between the individual canisters inside the same tunnel have been conservatively neglected. Furthermore, the system of tunnels and caverns has been simplified due to the geometry of the repository. Only one tunnel is considered in the 2- and 3D model studies.

The lateral boundaries (lines A-B and A'-B' in figure 3) represent the symmetry axes between the parallel, neighboring tunnels.

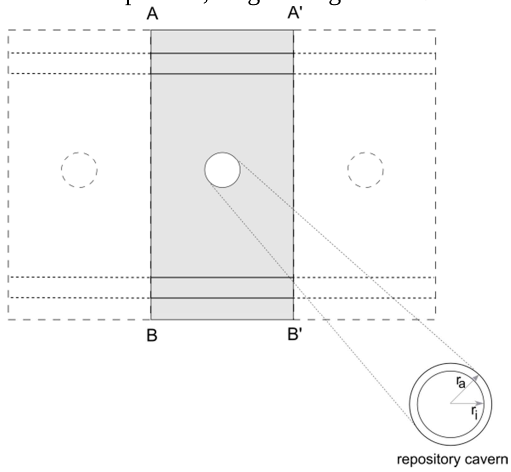

Figure 3: Sketch (not to scale) of the Geometry of a model that considers the host rock and its confining units. The gray area represents the model domain, the dashed areas show the neighboring caverns. The modeled area is defined by means of lateral symmetry axes.

In vertical direction, the model contains the host rock and in some cases, several confining units have been considered as well. The resulting doses were calculated directly at the boundaries of the host rock formation or the confining units respectively, conservatively disregarding any possible nuclide retention of other than the considered confining units.

3. Use of COMSOL Multiphysics

COMSOL's interfaces "Darcy's Flow" and "Solute Transport" for porous media were used to model the transport of radionuclides. Some important model parameters are compiled and listed in the appendix.

3.1 Groundwater Flow

Hydraulic potentials that govern the advective part of the transport were computed with the "Darcy's Law" module. The mass conservation of water is given by:

$$\frac{\partial}{\partial t}(\rho_f \phi) + \nabla \cdot (\rho_f u) = Q_m \qquad (1)$$

where ρ_f [kg m^{-3}] is the density of water, ϕ [-] is the porosity of the medium (full saturation is assumed), Q_m [kg (m^{3}s)$^{-1}$] is a fluid source/sink term and u [m s^{-1}] represents the Darcy velocity, that is defined by Darcy's Law according to:

$$u = -K\nabla h \qquad (2)$$

where K [m s^{-1}] is the hydraulic conductivity and h [m] the hydraulic potential.

As the hydraulic conditions are assumed to be stationary in this model, the term: $\partial/\partial t\ (\rho_f\ \phi)$ is equal to zero. Moreover, no additional fluid source or sink terms are assumed in this model. Hence, equation 1 can be simplified to give:

$$\nabla \cdot \rho_f(-K\nabla h) = 0 \qquad (3)$$

The vertical component of the hydraulic gradient ∇h is assumed to be 1m/m, the horizontal component is constrained to 0 m/m, which is implemented by applying according boundary conditions for the hydraulic potentials. Interactions between neighboring tunnels are taken into account by applying "no flow" lateral boundary conditions.

3.2 Radionuclide Transport

Comsol's "Solute Transport" module is used to calculate the time dependent radionuclide concentration, c, which is governed by diffusion, dispersion and sorption as well as by an advective flow component. The mass conservation equation is given by:

$$\frac{\partial}{\partial t}(\theta c) + \frac{\partial}{\partial t}(\rho_b c_p) + \nabla \cdot (cu) - \nabla \cdot [(D_D + D_e)\nabla c] = \sum (R + S) \qquad (4)$$

with:

θ [-]: volume fraction of the fluid

c [kg/m^3]: concentration of the nuclide in the fluid phase (mass nuclide per volume fluid)

ρ_b [kg/m^3]: bulk density of porous medium, i.e. $\rho_b = (1-\theta)\rho_p$, where ρ_p = particle density

c_p [kg/kg]: concentration of nuclide sorbed to solid phase (mass nuclide per mass solid phase)

D_D [m^2/s]: dispersive component of the hydro-dynamic dispersion tensor

D_e [m^2/s]: effective diffusive component of the hydro-dynamic dispersion tensor

R [kg/(m^{3}s)]: reaction rate of nuclide in the solid and fluid phase (in this case: radioactive decay)

S [kg/(m^{3}s)]: source term

The volumetric fraction of the fluid phase results from the porosity of the solid phase, ϕ, which is assumed to be constant over the whole domain of the porous medium, and the degree of saturation, s_f:

$$\theta = \phi s_f \qquad (5)$$

As a fully saturated porous medium is assumed (i.e. s_f = 1), the volumetric fraction of the fluid phase is the same as the porosity of the porous medium in this case.

The reaction rates, R, result from radioactive decay of the studied radionuclides in the solid and fluid phase:

$$R = -(\theta + \rho_b K_s)\lambda c \qquad (6)$$

with $K_s = c_p/c$ being the distribution coefficient for sorption of the radionuclide [m^3 kg^{-1}] and λ the according decay constant [s^{-1}].

Hence, equation 4 can be rewritten to yield:

$$\frac{\partial c}{\partial t}(\phi + \rho_b K_s) + \nabla \cdot (cu) - \nabla \cdot [(D_D + D_e)\nabla c] = -(\phi + \rho_b K_s)\lambda c + S \qquad (7)$$

S is the source term.

3.3 Source term, initial and boundary conditions

The source term represents the release of radionuclides after the containers have disintegrated. In the presented models, an instantaneous release of the radionuclides at t=0 has been conservatively assumed. The source term in this case has been implemented as an initial concentration of radionuclides inside the cavern. From here, the nuclides are released and decay during the transport process.

Fixed hydraulic potentials are applied to the vertical hydraulic boundaries, so that a vertical hydraulic gradient of 1m/m (flow direction upwards) is established throughout the whole model domain. Based on symmetry reasons, the lateral hydraulic boundaries are set to "no flow" in order to represent the interactions between parallel, neighboring tunnels.

Analogous, the lateral boundary conditions of the "Solute Transport" module are constrained to "no flux", whereas "zero concentration" conditions have been applied to the vertical boundaries.

4. Results

Figure 4 shows the resulting annual doses for model case (A) with host rock and confining units ("Brauner Dogger" including sandy limestones).

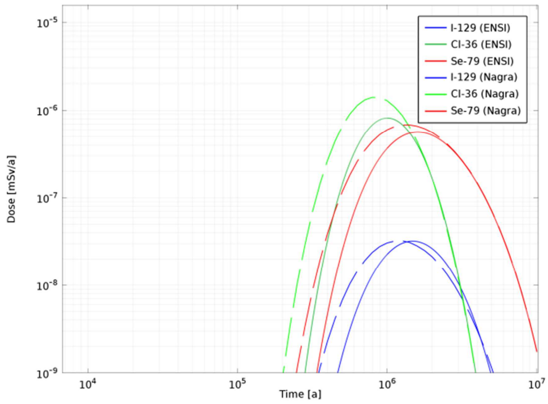

Figure 4: Resulting doses for model A that includes confining units. Solid lines are ENSI's results, dashed lines indicate results of the implementer Nagra. This model was calculated in 3D.

Resulting doses of a different model (B) with another waste type and the conservative assumption, that only the host rock itself – without confining units – is considered are shown in figure 5. The transport path length in that case was 20 m.

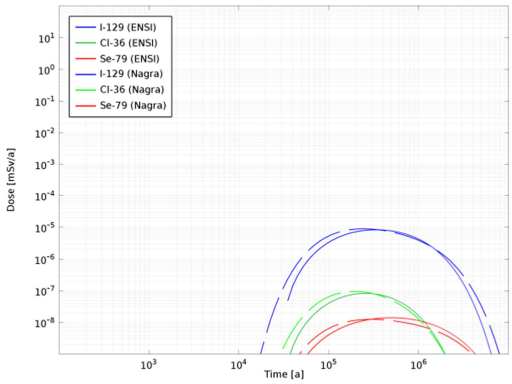

Figure 5: Resulting doses for the conservative model case B, where only the host rock itself has been considered (transport path length: 20m). Solid lines are ENSI's results, dashed line indicate results of the implementer Nagra. This model was calculated in 2D.

These doses were calculated from the integrated radionuclide flux across the model boundaries by means of biosphere transfer coefficients (NTB 08-05). Figures 6 and 7 show the evolution of the radionuclide concentration in the latter model B (20m transport path length; only the host rock; no confining units) after 10^5 and 10^7 years respectively.

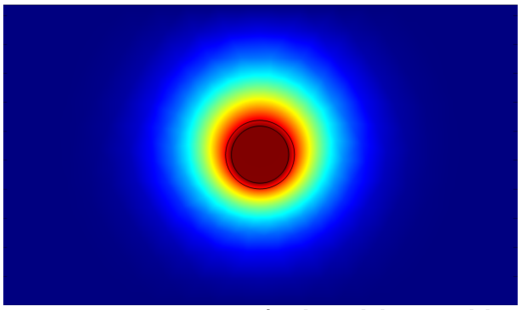

Figure 6: Concentration of radionuclide in model B after 10^5 years

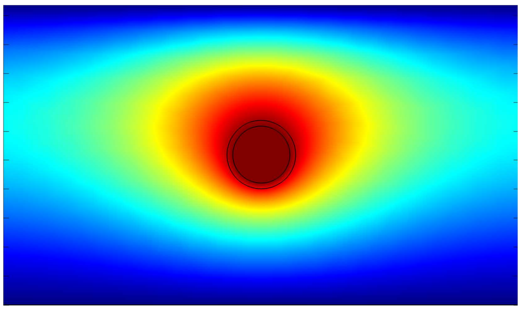

Figure 7: Concentration of radionuclide in model B after 10^7 years.

The doses calculated by the implementer (dashed lines in figures 4 and 5) are in the same order of magnitude as the doses yielded by ENSI's independent calculations. Differences between the calculated doses of ENSI and Nagra are most likely caused by different codes that were used.

5. Conclusions

COMSOL is a robust tool that has been and will be used by ENSI (among other codes) for radionuclide transport calculations in the technical and geological barrier systems of a geological repository. Special cases, such as the radionuclide transport in fault zones, are tasks that ENSI might calculate with COMSOL in future as well. Current work on this topic is in progress.

6. References

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7. Appendix

Table 1: Important nuclide specific material properties that were used in this study (Nagra (2008, 2010) and Kosakowski (2004)).

Parameter	Unit	I-129	Se-79	Cl-36
Molecular diffusion coefficient D_0	$m^2\ a^{-1}$	1.89E-3	1.89E-3	1.89E-3
Decay constant	a^{-1}	4.41E-8	6.3E-7	2.31E-6
Halflife $T_{1/2}$	a	1.57E7	1.1E6	3E5
Near field				
Effective porosity	-	0.2	0.2	0.2
Effective diffusion coefficient D_e	$m^2\ s^{-1}$	2E-10	2E-10	2E-10
Distribution coefficient for sorption K_s	$m^3\ kg^{-1}$	1E-3	3E-2	5E-3
Opalinus Clay				
Effective Porosity	-	0.06	0.06	0.06
Effective diffusion coefficient D_e	$m^2\ s^{-1}$	1.0E-12	1.0E-12	1.0E-12
Distribution coefficient for sorption K_s	$m^3\ kg^{-1}$	0.0	0.0	0.0
“Brauner Dogger”				
Effective Porosity	-	0.05	0.05	0.05
Effective diffusion coefficient D_e	$m^2\ s^{-1}$	2.0E-12	2.0E-12	2.0E-12
Distribution coefficient for sorption K_s	$m^3\ kg^{-1}$	0.0	0.0	0.0
“Sandy limestones”				
Effective Porosity	-	0.025	0.025	0.025
Effective diffusion coefficient D_e	$m^2\ s^{-1}$	7E-13	7E-13	7E-13
Distribution coefficient for sorption K_s	$m^3\ kg^{-1}$	0.0	0.0	0.0

Table 2: Inventory of studied radionuclides in models A and B (unpublished Nagra internal report (2011)).

Model	I-129	Se-79	Cl-36
A	2.29E8 [Bq]	3.3 E11 [Bq]	7.9E12 [Bq]
B	4.92E10 [Bq]	3.04E9 [Bq]	6.46E10 [Bq]