

## MODELLING OF RESATURATION, GAS MIGRATION AND THERMAL EFFECTS IN A SF/ILW REPOSITORY IN LOW-PERMEABILITY OVER-CONSOLIDATED CLAY-SHALE

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### ABSTRACT

Radioactive wastes conditioned for final disposal in repositories in deep, low permeability formations will produce a significant amount of gas due to corrosion and microbiological degradation processes. This paper addresses the process of gas release from disposal tunnels for spent fuel (SF) and long-lived intermediate level wastes (ILW) in a clay-shale formation. For the SF the impact of additional heat transfer is considered. The issues under consideration are the interference of the repository resaturation process by the build-up of gas pressures in the disposal tunnels and the impact of waste-generated thermal loads on fluid and gas flow.

Numerical simulations were conducted, representing the backfilled disposal tunnels (SF and ILW, respectively) and the surrounding host rock formation by a two-dimensional cross-section. The simulations were carried out with the TOUGH2 EOS5 module.

The paper gives results of a sensitivity study, aimed at investigating the impact of repository-induced processes (heat, gas generation) and parameter uncertainties on the evolution of porewater pressure in the backfilled disposal tunnels. The numerical simulations are of an indicative nature and did not make use of the final reference values for NAGRA's demonstration project of SF/HLW/ILW disposal feasibility in the Opalinus Clay formation.

### INTRODUCTION

The Swiss National Cooperative for the Disposal of Radioactive Waste (NAGRA) has submitted by the end of 2002, three reports on the demonstration of disposal feasibility for spent fuel (SF), vitrified high-level waste (HLW) and long-lived intermediate-level waste (ILW) in the Opalinus Clay (Nagra 2002a,b,c) to the Swiss safety authorities.

Figure 1 presents schematic cross-sections of Swiss SF / HLW / ILW emplacement tunnels in the clay formation (after Nold 2000). The SF, HLW and long-lived ILW are emplaced in separate tunnels (HLW is not treated in the present study). The SF in steel

canisters will be arranged in a row, separated by a distance of 3 m, along small-diameter tunnels, embedded in a bentonite buffer. The ILW containers will be placed in two tunnels. The ILW tunnels will be backfilled with cementitious mortar and then sealed with a concrete plug.

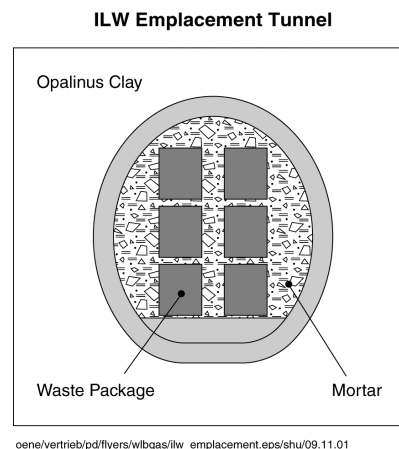
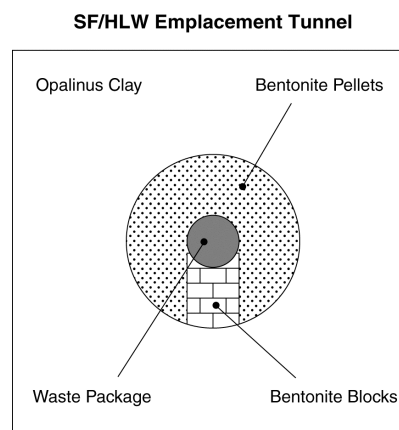


Figure 1. Schematic view of the Swiss proposed layout for a SF / HLW/ILW repository in a sedimentary host rock (after Nold 2000).

The following questions concerning long-term behavior of the system have been investigated by means of numerical simulations:

- What is the maximum gas pressure expected in SF and ILW disposal tunnels during the gas generation phase?
- How is the gas pressure expected to develop with time and when will a quasi-stationary gas flow be reached?
- Subsequent to closure of the repository, how does the resaturation process interfere with gas accumulation in an ILW disposal tunnel?
- Does heat production of SF affect build-up of gas pressures in the SF disposal tunnels?

Assessment of processes during the post-closure period of the repository includes:

- resaturation of backfilled drifts
- gas dissolution in the pore water (Henry's law)
- gas migration into backfill materials and rock under the assumption of multiphase flow in an homogeneous porous medium
- pore water displacement and
- thermal conduction and expansion.

A simplified representation of the SF and ILW disposal tunnels was used, considering a 2-D vertical plane with a vertical symmetry axis in the middle of the tunnel. The numerical simulations were conducted with the TOUGH2 EOS5 module, offering the following features:

- constant (SF) or time-dependant (ILW) gas source (hydrogen only)
- time-dependant heat source (SF only)
- solubility of gas in water (Henry's law)
- flow and thermo-physical properties (single and two-phase) of backfill materials and host rock.

### **MODEL DESCRIPTION**

For reasons of simplification, only one meter length of a tunnel is modelled. Due to symmetry conditions, a vertical cut through the host rock and the emplacement tunnel is considered. A further symmetry condition is given for the SF tunnels, because they are arranged in a panel of parallel tunnels with separation distances of 40 m.

Concerning the ILW tunnel, the horizontal extension of the model domain is 50 m (distance from the symmetry axis).

The model domain has a vertical extension of 130 m. Fixed pressure boundaries are assigned to the top and the bottom of the model, simulating the presence of water conducting features in overlying and underlying confining units.

The ILW tunnel with a radius of 3.5 m is discretized as an equivalent rectangular area. The SF tunnel with a radius of 1.25 m contains a source element in which gas and heat production is located (equivalent to the container radius of 0.5 m).

Both models are discretized with a total of 1,175 finite volumes. Figure 2 illustrates as an example the ILW model discretization

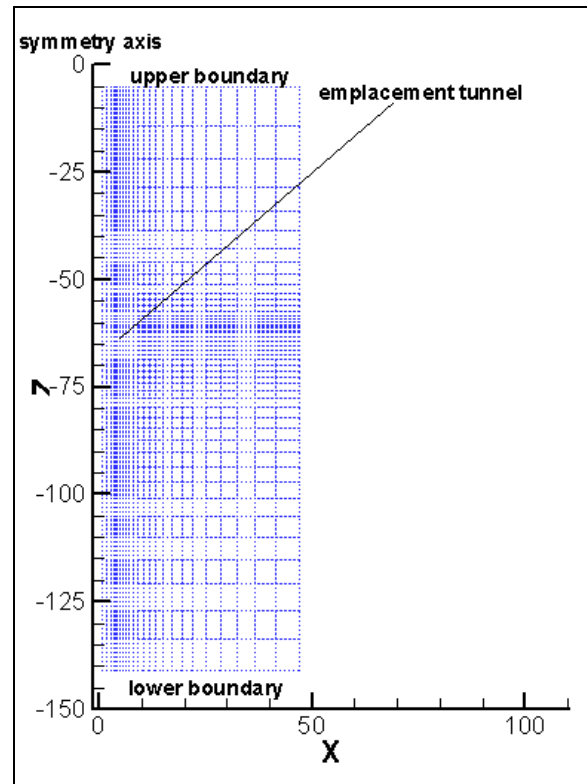


Figure 2. Discretization of the ILW model

The main parameters used for the simulation are given in Table 1.

Table 1. Parameter set used for the simulations

	Clay	Mortar (ILW)	Ben-tonite (SF / HLW)	Units
Grain density	2,540	2,490	2,700	kg/m <sup>3</sup>
Porosity $\phi$	0.12	0.24	0.52*	-
Permeability	10 <sup>-20</sup>	10 <sup>-18</sup>	10 <sup>-19</sup>	m <sup>2</sup>
Thermal conductivity	2.50	-	1.35	W/m K
Specific heat	905	-	964	Ws/kg K
Rock compressibility ( $\alpha/\phi$ )	1.83·10 <sup>-9</sup>	2.5·10 <sup>-10</sup>	3.58·10 <sup>-9</sup>	Pa <sup>-1</sup>
Thermal expansion	3.47·10 <sup>-5</sup>	-	1.5·10 <sup>-5</sup>	K <sup>-1</sup>
Residual liquid saturation	0.5	0.5	0.3	-
Initial liquid saturation	1.0	0.2	0.3	-
Residual gas saturation	0.0	0.0	0.0	-
van Genuchten coefficient	1.67	2	1.82	-
Gas entry pressure	1.8·10 <sup>7</sup>	1·10 <sup>5</sup>	1.8·10 <sup>7</sup>	Pa

\* enhanced porosity was used to account for low emplacement densities of the backfill (bentonite pellets)

Several of the material properties given in Table 1 depend on the actual water content of the medium (e.g. thermal conductivity of bentonite, rock compressibility, porosity). However, the water saturation of the backfill materials and of the host rock changes during the resaturation process. Such parameter uncertainties were addressed by parameter variations. In particular, a sensitivity study to the hydraulic diffusivity of the host rock and on the gas production rate was performed.

**INITIAL AND BOUNDARY CONDITIONS**

Hydrostatic conditions with a porewater pressure of 7.5 MPa at repository level are assumed as initial conditions. The top and the bottom of the model are maintained at constant pressures. A two year period of operation of the SF tunnels and a four year period of the ILW tunnels under almost atmospheric conditions results in a near field depressurization. Figure 3 illustrates the pressure in the modeled area in the post closure period.

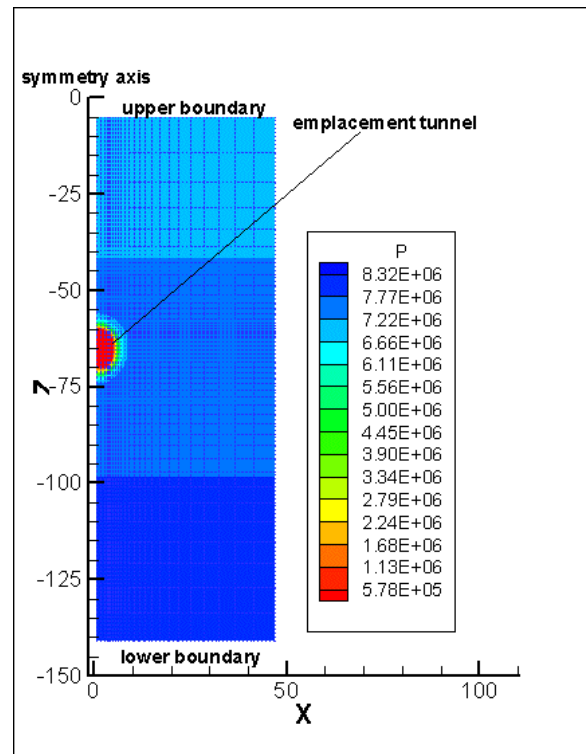
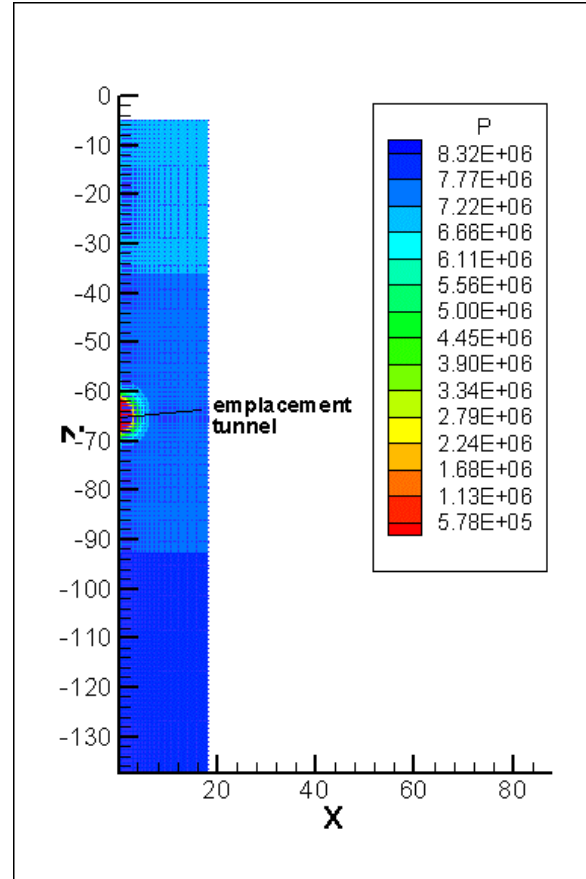


Figure 3. Initial conditions for the pressure (in Pa) after operation (SF top, ILW bottom)

Gas generation in the SF tunnels is mainly due to the corrosion of carbon steel, which results in  $H_2$ -production. Given the total amount of steel to be emplaced in the HLW tunnels and assuming conservative estimates of steel corrosion rates of 1 - 10  $\mu\text{m}/\text{year}$ , the expected average gas production rate is 1.5 to 15 mol  $H_2$  per m tunnel length and year (0.04 to 0.4  $\text{m}^3 \text{ gas}_{\text{STP}}$  per  $\text{m}^3$  waste and year).

Gas generation in the ILW tunnels arises from corrosion of steel, zircaloy and aluminum. In addition, degradation of organic materials will contribute with the production of  $CH_4$ . Figure 4 illustrates the expected range of gas production in the ILW tunnels.

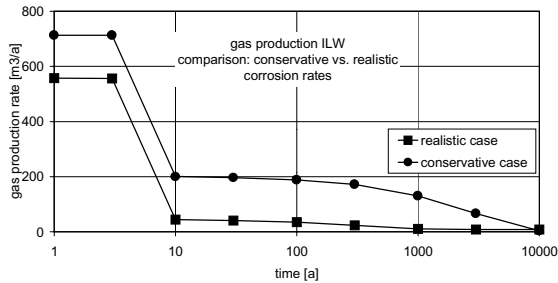


Figure 4. Total gas production rates expected in the ILW tunnels (Nagra, 2002)

For the thermal investigations, a reference SF canister ( $UO_2$  and MOX assemblies) with an initial thermal output of 1,500 W was considered. The heat production of the canister declines over time (Figure 5).

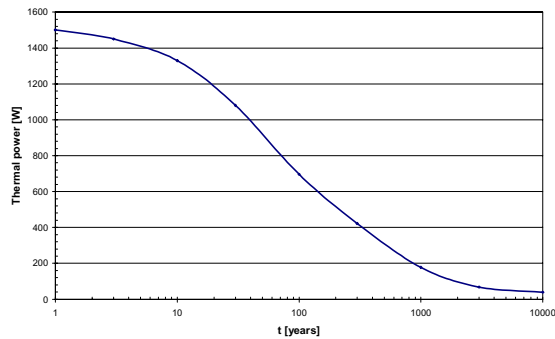


Figure 5. Thermal power of a SF container (McGinnes, 2002)

## Results

### Re-saturation

The re-saturation of the ILW tunnel is found to be highly dependent on the hydraulic diffusivity of the host rock and on the porosity of the backfill material. At reference conditions (Table 1) the tunnel is completely saturated after a period of about 1,000 years. Figure 6 presents the water saturation at different horizontal distances from the tunnel centre and within the backfill materials. The 2.5m-curve is the mortar-element next to the host rock.

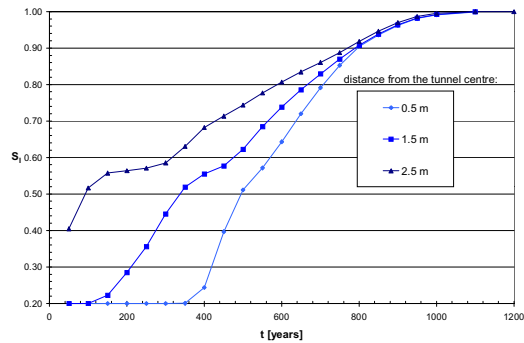


Figure 6. Resaturation of the ILW disposal tunnel (reference conditions)

The Figures 7 illustrates the liquid saturation and pore water velocities in the vicinity of the ILW disposal tunnel and at selected times after closure (immediately after closure, 50 years, 100 years, 500 years). Parametric studies indicate that hydraulic diffusivity is the determining factor for the resaturation time of the ILW disposal tunnels.

The resaturation of the SF tunnels is shown to be much faster due to the smaller tunnel pore volume. In addition, the numerical simulations give evidence for enhanced saturation due to thermal effects (The pore volume of  $0.83\text{m}^3/\text{m}$  cavern length will be saturated after about 40 years compared to 145 years under isothermal conditions). The Figures 8 illustrates the temperature ( $T$  [ $^{\circ}\text{C}$ ]), the liquid saturation (SL) and the pore water velocities in the tunnel and the surrounding rocks at two selected times (5 years and 50 years, respectively). The simulations were based on the reference data set, given in Table 1.

The heat emitted into the host rock is found to increase the pore pressure in the surrounding host rock over a period of 50 years, accelerating re-saturation, as illustrated in Figure 9.

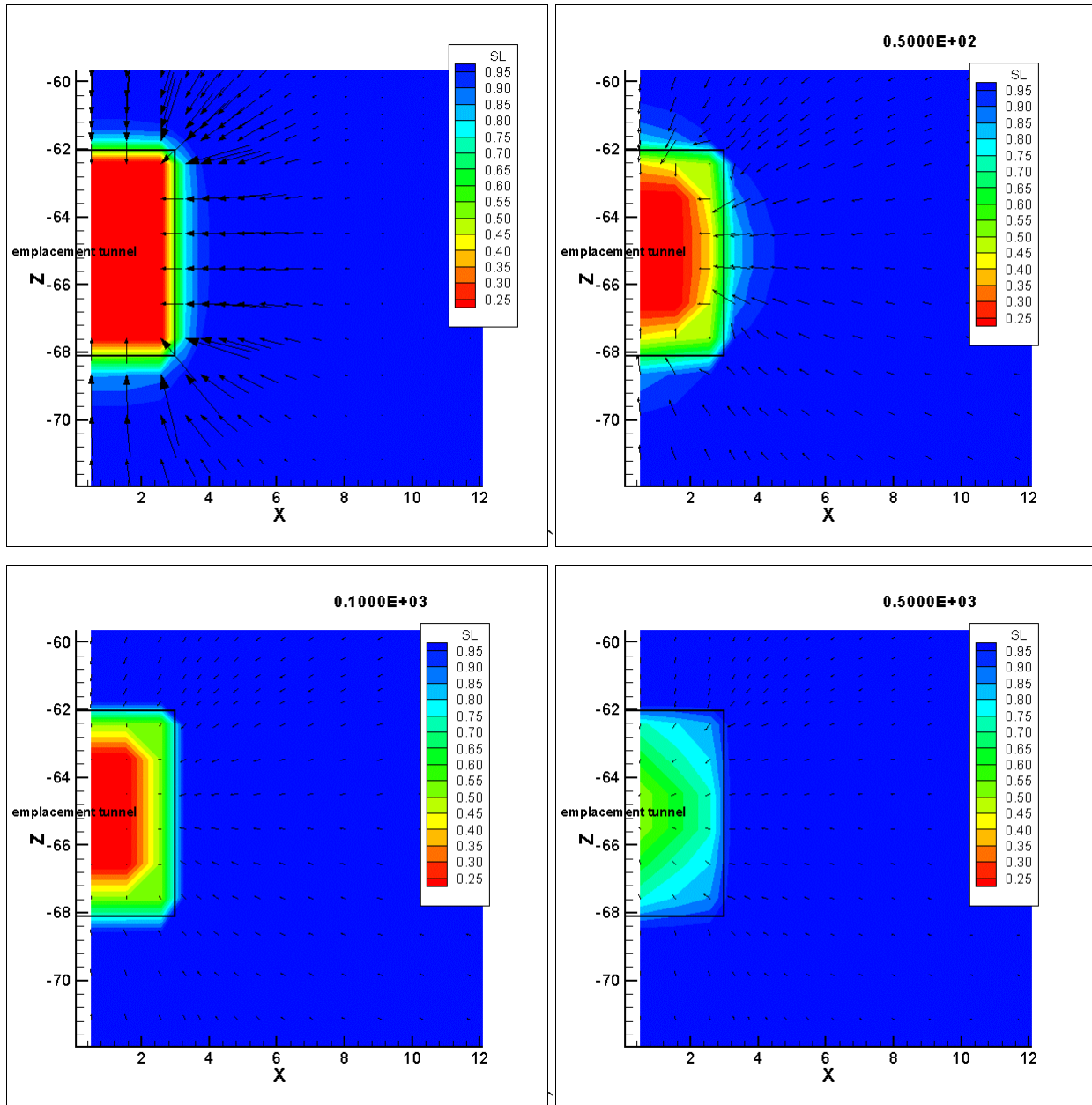


Figure 7. Resaturation of the ILW disposal tunnel: immediately after closure (top left), 50 years after closure (bottom left), 100 years after top right (left) and 500 years after closure (bottom right)

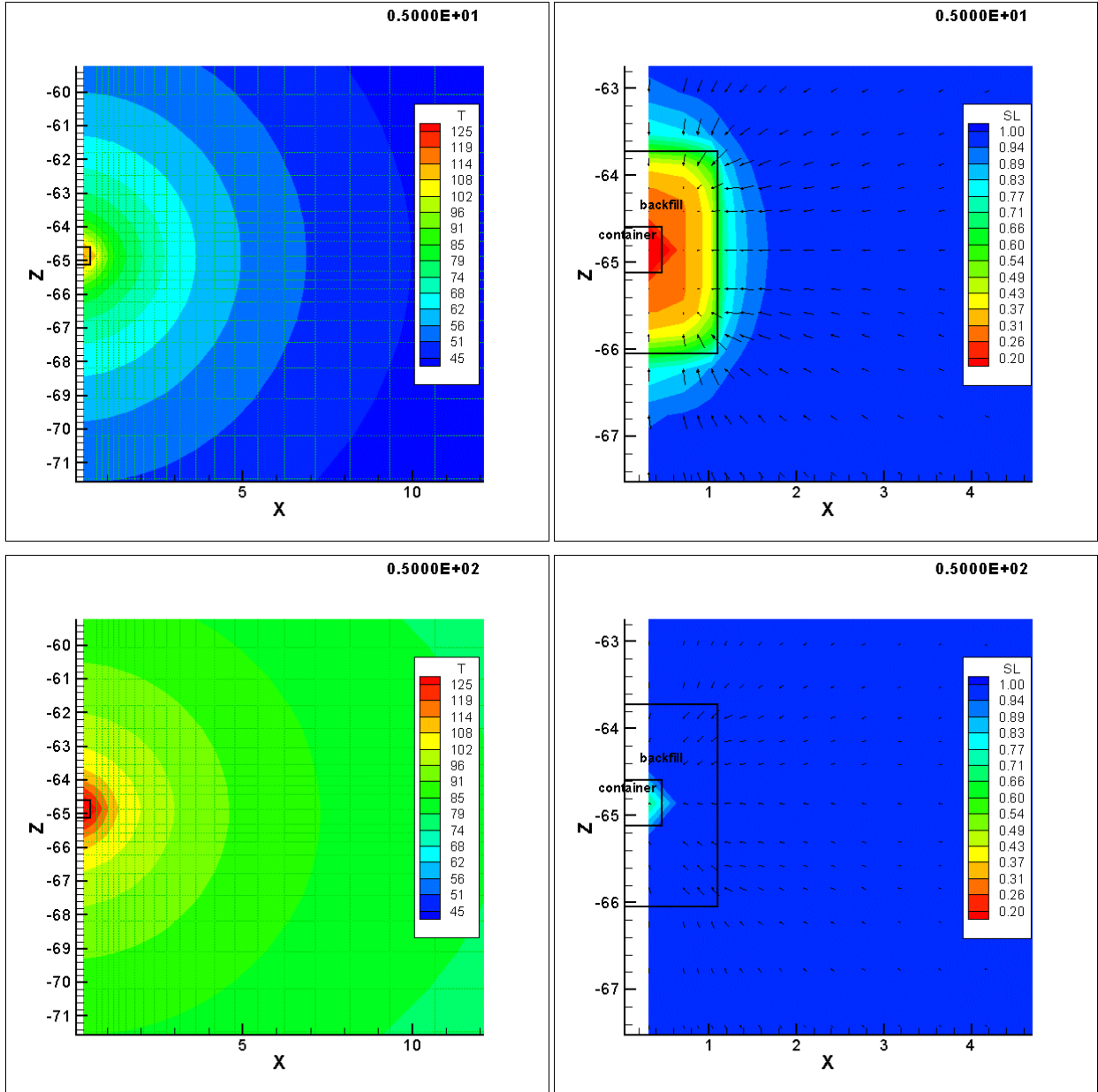


Figure 8. Non-isothermal resaturation of the SF tunnel: 5 (left) and 50 years (right) after closure (top: temperature, bottom: water saturation / detail )

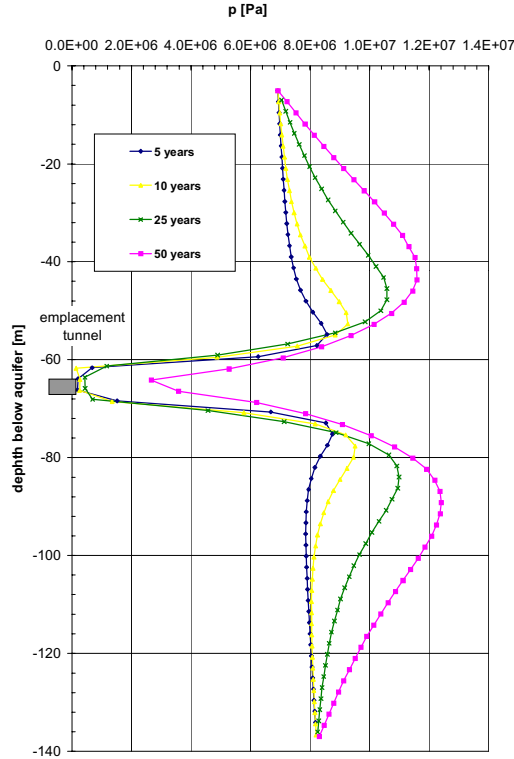


Figure 9. Pressure evolution during resaturation

As the resaturation progresses, capillary pressure of the bentonite backfill decreases rapidly (Figure 10) and the role of suction pressure of the bentonite becomes negligible. Eventually, the resaturation is largely determined by the porosity of the backfill and by the hydraulic diffusivity of the host rock.

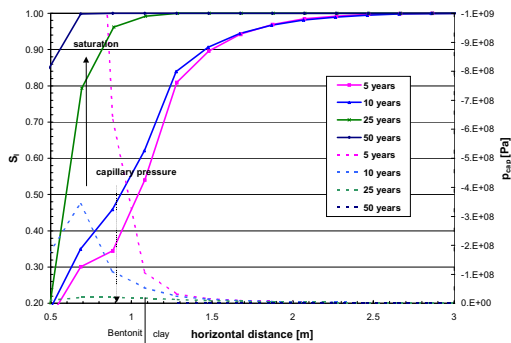


Figure 10. Capillary pressure (dashed lines) and saturation in the nearfield zone

Given the range of parameters assessed in this study, the resaturation of the SF tunnels may take a time period between 50 and 400 years. The simulations indicate that heat production accelerates the saturation process. This result may be explained by

the fact that thermal diffusivity is about 30 times higher than the hydraulic diffusivity - the heat pulse propagates faster than the hydraulic disturbance, which causes a thermally induced hydraulic gradient towards the disposal tunnel. In addition, the dependency of fluid viscosity on temperature causes an increase of hydraulic conductivity in the vicinity of the tunnel.

### Gas production and migration

Different cases were simulated based on different gas production schemes. Concerning the ILW tunnel, time-dependent production rates have been considered (cf. Figure 4), assuming that the onset of gas production is immediately after repository closure, after 50% resaturation of the disposal tunnel and after full resaturation. For the SF tunnel, a constant gas production rate is assumed, but the impact of heat emission has been investigated.

For an ILW tunnel, Figure 11 summarizes the simulations of the long term pressure build-up for the different gas production schemes. Although, the pressure build-up is found to depend on the different production rates (realistic and conservative) and, to a lesser extent, on the starting conditions, even at conservative gas production rates the porewater pressure in the tunnel does not exceed 12 MPa - this is about 4.5 MPa above the steady state hydrostatic pressure at repository level. The pressure build-up is governed by the hydraulic properties of the host rock rather than by its two-phase flow parameters. On the other hand, the total system compressibility (composite effect of mortar compressibility and host rock compressibility) is relevant. Water is expelled from the tunnel into the host rock formation due to the increasing pressure, creating new storage volume for the gas in the tunnel. The amount of gas, entering the host rock is low during the entire phase of overpressurisation.

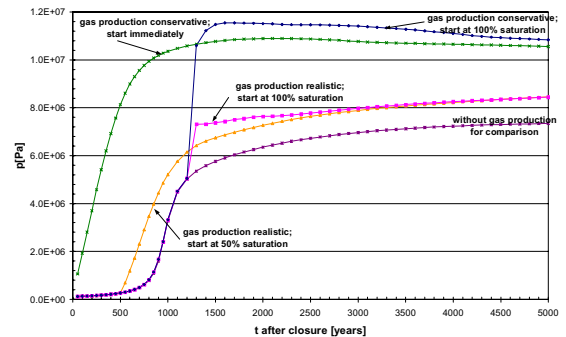


Figure 11. Long-term pressure build-up in the ILW disposal tunnel

Figure 12 illustrates the effect of the heat emission of the SF on the pressure build-up at early times. Build-up of pore pressure is governed by the thermo-hydraulic processes in the host rock. Thermal expansion creates significant overpressures during the first 300 years. Decreasing temperature at late times leads to thermal contraction - the pore pressure drops below the baseline, corresponding to isothermal conditions. On top of this thermo-hydraulic mechanism, gas production may shift pressure build-up by 3 - 5 MPa.

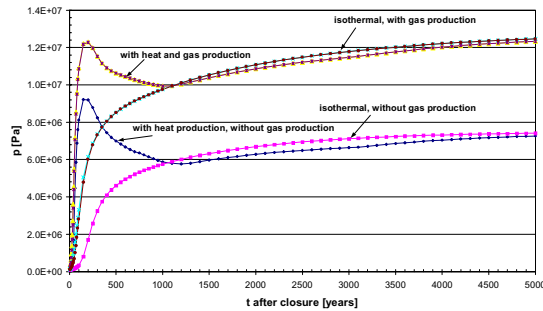


Figure 12. Long-term pressure build-up in the SF / HLW tunnel considering different production processes

## CONCLUSION

This sensitivity study was aimed at investigating the impact of repository-induced processes (heat, gas generation) and parameter uncertainties on the evolution of porewater pressure in the backfilled disposal tunnels for SF and ILW of a repository in the Opalinus Clay formation. The following conclusions are drawn:

- The resaturation of the disposal tunnels is dominated by the hydraulic diffusivity of the host rock formation and by the porosity of the backfill materials. For ILW the estimated resaturation time is in the order of about 1,000 years and for SF several 100 years.

- Pressure build-up due to gas generation may cause excess pressures in the disposal tunnels in the order of 3 - 4 MPa. Hydraulic conductivity of the host rock and system compressibility of the disposal tunnels are the determining factors for the expected peak pressures.
- Heat production in the SF tunnels in combination with gas production may lead to excess pressures of up to 5 MPa. However, the effect of the heat pulse is expected to disappear after several hundred years.

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