Modelling the Thermal Impact of a Repository for High-Level Radioactive Waste in a Clay Host Formation

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Abstract: High-level radioactive waste can generate considerable amounts of heat as a side effect of radioactive decay. This paper shows how Comsol Multiphysics has been used to evaluate the physical impacts of the heating of the geological media around a deep disposal system. Comsol Multiphysics was found to be well suited to the simulation of the relevant processes at the large time and spatial scales that are common to geological disposal system studies.

Keywords: radioactive waste, geological disposal, thermal, modelling.

1. Introduction

In all nuclear power generating countries, spent nuclear fuel and long lived radioactive waste management is an important environmental issue today. Disposal in deep clay geological formations is one of the promising options to dispose of these wastes.

The Belgian radioactive waste management programme has, since 1976, focused on the geological disposal of high-level and long-lived waste in clay formations; the Boom Clay layer is studied as reference formation [1].

A typical layout for a geological repository in clay is shown in Figure 1. The proposed repository will have a central access facility consisting of at least two vertical transport shafts and one main transport gallery. The disposal galleries will be excavated perpendicular upon the transport gallery.

As a side effect of radioactive decay, high-level radioactive waste and spent fuel generate considerable amounts of heat. When those waste types are disposed in a geological repository located in a clay formation, the generated heat will cause an increase of the temperature of the engineered barriers, the host clay formation and the surrounding geological layers. The amount of radioactive waste per gallery and the spacing between galleries have to be adapted to the thermal output of the waste.

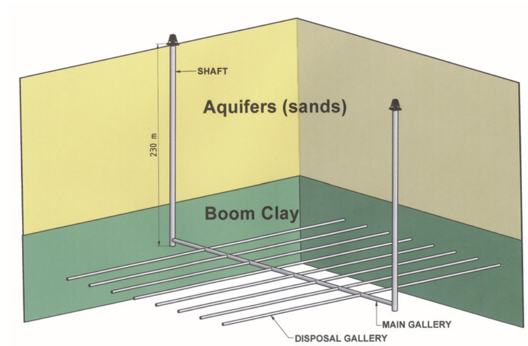

Figure 1. Typical repository layout.

The thermal evolution of a deep repository for heat-emitting radioactive waste affects many aspects of geological disposal. Among these aspects are the thermo-hydro-mechanics of the host formation and engineered barriers, but also the chemical conditions in the vicinity of the waste packages and the geochemistry throughout the host formation, which condition degradation rates of the waste forms and the migration parameters of dissolved species respectively. The far field temperature evolution could also be an important facet of the environmental impact assessment [2]. In this paper, we focus on the latter, through computation of the thermal impact of the repository on its far field and, as a consequence, the possible uplift of the ground above.

2. Heat transport and thermal impact

2.1 Source term

The residual heat dissipated by vitrified high level waste (VHLW) per equivalent ton of reprocessed heavy metal (tHM) can be directly calculated from the radionuclide inventory of the waste as the specific activity and the thermal energy released by disintegration are fairly well-known for the main radionuclides that contribute to the production of heat. Among others, the ORIGEN code [3] can be used to that effect. A good estimate of the heat production as function of time can also be obtained by fitting the results of waste decay computations with a formula of the type:

$$Q = \sum_i A_i \, e^{(-b_i t)} \quad (1)$$

where t is defined as the time elapsed since the production of the waste. A set of values of the coefficients A_i and b_i was derived by Put [4] for vitrified waste arising from the reprocessing of spent fuel with a burn-up of 33 GW×day/tHM. These values are given in Table 1. In Figure 2, the heat release according to Put's formula is compared with the results of a full calculation with ORIGEN.

Table 1: Source term coefficients for Eq. (1)

A_1 (W/tHM)	**A_2**	**A_3**	**A_4**
5021	1205	27.04	0.7576
b_1 (1/year)	**b_2**	**b_3**	**b_4**
0.3894	0.02458	1.63×10^{-3}	6.55×10^{-5}

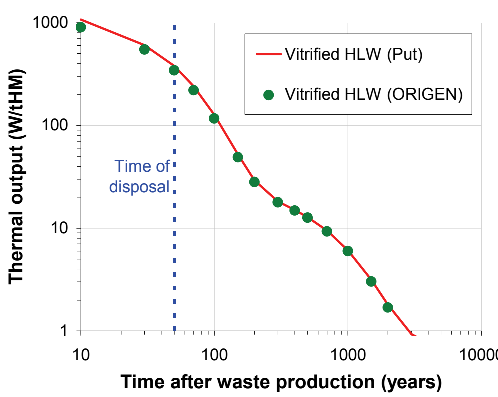

Figure 2. Source term.

For the currently studied disposal options, it is planned to let the VHLW cool in surface facilities during a few tens of years, taking advantage of the decay of several relatively short-lived nuclides to limit the thermal load at the time of disposal. In the considered design, one metre of disposal gallery will contains, on average, waste produced by the reprocessing of about 0.63 tHM after 50 years of cooling. The linear thermal load density will thus be about 240 W/m of gallery at the time of disposal.

2.2 Heat transport through the host clay layer

In the host clay layer, heat transport is essentially diffusive, *i.e.* occurs through conduction only as the very low permeability of clays prevents significant groundwater flow. The transport of heat is thus simply written as

$$\frac{\partial}{\partial t}\left(\rho_b \, c_{p,b} \, T\right) = \nabla \cdot \left(\lambda \nabla T\right) \quad (2)$$

in which T is the temperature, λ the thermal conductivity and $\rho_b \, c_{p,b}$ is the bulk thermal capacity per unit volume of saturated porous media, *i.e.*

$$\rho_b \, c_{p,b} = \eta \, \rho_w \, c_{p,w} + (1-\eta) \, \rho_s \, c_{p,s} \quad (3)$$

where η is the porosity of the clay media, ρ_w , ρ_s and $c_{p,w}$, $c_{p,s}$ are the densities and thermal capacities of groundwater and the solid phase.

2.3 Heat transport in the aquifers

In the aquifers, advection and possibly convection can occur as the permeability is large enough for small density gradients to induce significant flows [5].

To take advection and convection into account, the evolution of the temperature and velocity fields have to be modelled in parallel, leading to the coupled partial differential equations system

$$\frac{\partial}{\partial t}\left(\rho_b \, c_{p,b} \, T\right) + \nabla \cdot \left(\rho_w \, c_{p,w} \, T \, \mathbf{u}\right) = \nabla \cdot \left(\lambda \nabla T\right) \quad (4)$$

$$\frac{\partial}{\partial t}\left(\eta \, \rho_w\right) = \nabla \cdot \left(\rho_w \, \mathbf{u}\right) \quad (5)$$

$$\text{with } \mathbf{u} = \frac{k}{\mu}\left(\nabla p - \rho_w \, \mathbf{g}\right) \quad (6)$$

in which $\mathbf{u}$ is the vector of Darcy velocities.

Equation (4) stands for the conservation of heat as it is transported by the flowing groundwater and conduction. Equation (5) describes the conservation of mass: if the divergence of the mass flux density (RHS of 5) is non-zero, the excess or default mass has to be accommodated by local changes of pore volume η and fluid density ρ_w (LHS of 5). Equation (6) is the Darcy law, in which k [m^2] is the intrinsic permeability of the porous medium, μ [Pa•s] is the temperature-dependent dynamic viscosity of the groundwater, ∇p [Pa/m] is the pore pressure gradient and $\mathbf{g}$ [m/s^2] is the gravity vector. The link from the flow to the heat transport equation is $\mathbf{u}$, while the link from the heat transport back to the flow equation is given through the dependency of ρ_w and μ, hence $\mathbf{u}$ on temperature.

2.4 Comsol Multiphysics model

For a first series of calculations aimed at determining what the maximum increase of temperatures in the clay could be, it was conservatively assumed that no flow occurs through the surrounding aquifers. As heat transport is, in this case, purely conductive, the 3D problem can be simplified as shown in Figure 3.

Assuming that the thermal source term is uniform along the length of several parallel, horizontal disposal galleries, the largest temperature increases should be encountered in a vertical plane perpendicular to the axes of the galleries, crossing these galleries at mid-length. If the length of the disposal galleries is large compared to the thickness of the host formation, the temperature field in that plane should not differ much from the one computed in three dimensions, as if the galleries were of infinite length, because the impact of a better dissipation at the ends of finite galleries will have little effect on the temperature near the centre of the repository. Moreover, the problem can be reduced to the transport of heat around a single gallery, the interactions between an infinite number of adjacent galleries being introduced through "no heat flux" Neumann-type boundary conditions across parallel vertical planes at mid-distance between two galleries as shown in Figure 3a and 3b. Again, this is a conservative approximation as the enhanced heat dissipation at the edges of a repository system with a finite number of disposal galleries is neglected. Finally, the model can be further reduced by taking advantage of the symmetry of the problem along the vertical plane of the gallery through an additional "no heat flux" Neumann-type boundary condition.

In the vertical direction, the model geometry is bounded by the ground surface assumed to be located about 220 metres above the plane of the repository.

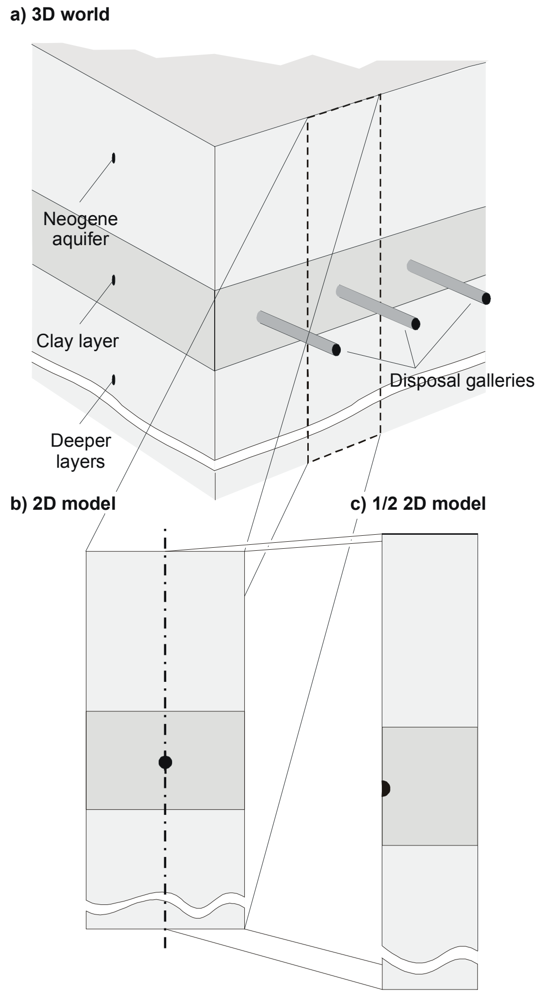

Figure 3. Model reduction (only in the absence of groundwater flow). Not to scale.

However, no strict depth limit for the model can be set a priori as the problem is semi-infinite. The model was thus arbitrarily limited to a depth of 800 meters under the repository, corresponding to a total depth of 1020 m. It was subsequently verified during the calculations that this is deep enough, as the temperatures obtained by prescribing a Neumann-type "no heat flux" or Dirichlet-type "no temperature variation" condition at the bottom boundary do not differ by more than 0.25 °C within the Boom Clay.

In a second set of calculations, the effects of groundwater flowing through the Neogene aquifer above the clay were investigated. A two-dimensional model is used, which can be represented by a slice perpendicular to the galleries in Figure 2. The model now includes all eight galleries planned for the disposal of

VHLW, as flow patterns in the upper aquifer cannot be limited to the region above a single gallery. For a purely thermal problem, the temperature increases could directly be computed, as was done in the first calculation set because that problem is linear. As equations (4)-(6) are coupled through densities and viscosities which are non-linearly temperature-dependent, absolute temperatures have to be used. Hence, the geothermal heat flux is ascribed as bottom boundary condition, a yearly average temperature of 10°C is fixed at the top and the existing geothermal gradient is used as initial condition. To highlight the perturbations that are induced by the presence of the disposal system, calculation results are still shown as temperature increases by subtracting the initial conditions from the simulation results

For some problems, the full system of equations (4)-(6) can be simplified. In particular, provided that the density variations are limited in the considered temperature range, these can be neglected in most terms except in the so-called buoyancy term ρ_w g of the Darcy equation (6). This is commonly referred to as the Boussinesq assumption. An intermediate simplification is to only use the Boussinesq assumption for the heat transport equation but not for the flow equation. The latter approach was adopted for this study, after comparison with the results obtained for a different repository configuration [4].

The thermal parameters used in the model are summarized in Table 2. As the focus of this study is on the far field temperatures, the source term was simply distributed homogeneously over the gallery area (r ≤ 1.6 m), where a relatively coarse mesh is used.

A nice feature of Comsol Multiphysics is that one can selectively disable the flow equations in the part of the domain corresponding to low-permeability clay, which significantly stabilizes and speeds up the simulations.

Table 2: Thermal parameters

Layer	λ (W m^{-1}K^{-1})	$\rho_b\, c_{p,b}$ (J m^{-3}K^{-1})
Boom Clay	1.35	2.90×10^6
Neogene aquifer	2.05	2.84×10^6

2.4 Results of heat transport calculations

Typical vertical temperature profiles and evolutions of temperature obtained from the first, conservative, calculation set are shown in Figures 4 and 5.

At the top of the Boom Clay, the increase of temperature is less than 12°C and the peak temperature there is reached about 150 years after disposal. The peak temperature in the upper part of the Neogene aquifer (between 20 m and 50 m depth) is reached after about 500 years and does not exceed a couple of degrees.

For the second set of calculations, groundwater flow was enabled in the Neogene aquifer above the clay and the relations

$$\rho = 1000.2 - 0.005 \times T^2 \quad [\mathrm{kg/m^3}] \qquad (7)$$

$$\mu = \rho \cdot 9.2\times10^{-7} \cdot \exp(2050/(273.15+T)) \quad [\mathrm{Pa \cdot s}] \qquad (8)$$

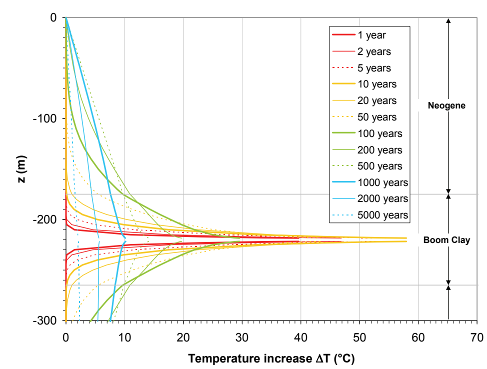

Figure 4. Computed profiles of temperature increase ΔT in the vertical plane of a disposal gallery if the disposal galleries are 50 m apart from each other.

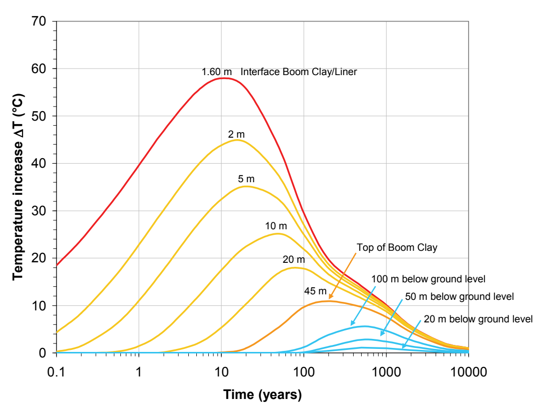

Figure 5. Time histories of temperature increase ΔT at various distances above a disposal gallery (orange) and below the ground level (blue).

in which T is in Celsius for temperature-dependent groundwater density ρ and viscosity μ were introduced in the model. These relationships provide a good fit of various tabulated experimental data in the temperature range 5°C - 60°C, which is much wider than the expected temperatures in the Neogene aquifer.

The Neogene aquifer is composed of several stratigraphical units [6]. For the simulations in this study, we considered a lumped value of the permeability $k = 2\times10^{-11}$ m^2 as representative for the whole Neogene aquifer. Combined with an average local hydraulic gradient of about 0.1%, this correspond to an average Darcy velocity $u_D = 6.3$ m/year, or an average pore velocity $u_p = 21$ m/year if a porosity $\eta = 0.30$ is assumed for the aquifer. In this study, we assume that the general flow direction is perpendicular to the galleries of the disposal system, which should provide a conservative estimate of the temperatures in the aquifer, above the downstream edge of the repository.

The effect of the assumed local flow pattern is shown in Figure 6, which gives the computed temperature field 200 years after the disposal of VHLW. The evolution of the temperature increase ΔT at selected points above the downstream edge of the repository is shown in Figure 7. This figure can be compared to the "no flow" case also shown in Figure 5. The addition of advective transport in the Neogene aquifer to the model clearly results in a better cooling of the Boom Clay and lower average temperatures in the aquifer as the thermal energy diffusing out of the clay is used to heat a larger volume of (flowing) water.

Although the model used can represent density-driven flow, the simulation does not predict the development of convection cells in this case. An additional simulation was thus performed with no base flow in the Neogene aquifer to investigate the possible development of thermal convection cells.

In absence of a natural hydraulic gradient, this constitutes a worst-case scenario in terms of heating the upper regions of the aquifer through rising hot plumes. The results of this simulation, shown in Figures 8 and 9, show the development of two convection cells above the eight disposal galleries. Figure 8 also indicates that the convection cells improve heat transport towards the top of the aquifer, but that their impact on the average temperatures in the aquifer is rather limited. In fact, the average temperatures in the aquifer and in the clay are lower than in the "no flow" case, as heat is effectively carried away from the repository by the circulation in the aquifer.

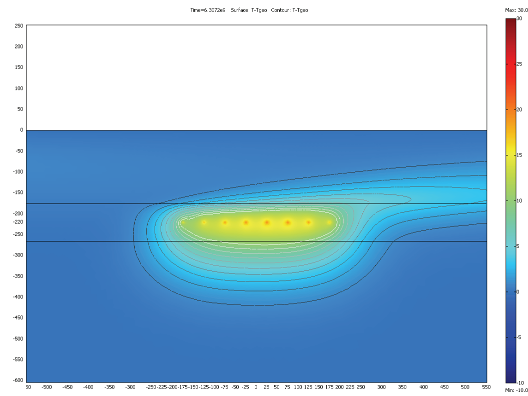

Figure 6. Temperature increase field ΔT, 200 years after the disposal of VHLW. The heat released from the clay is carried away by advection in the Neogene aquifer, which also enhances the cooling of the clay.

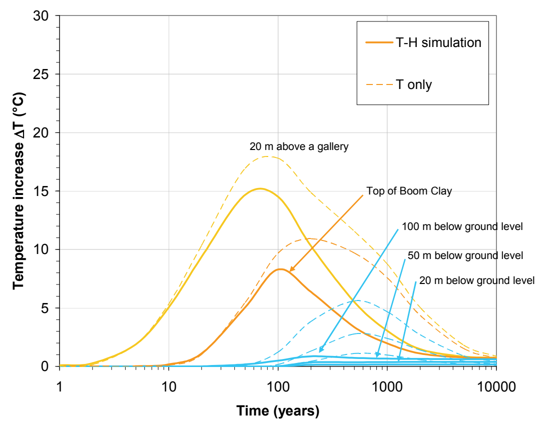

Figure 7. Time histories of temperature increase ΔT at various distances above the downstream disposal gallery (plain lines), compared to the results of the "no flow" case (dashed). The additional cooling due to water flowing through the aquifer is clearly visible.

3. Thermo-mechanical impact: uplift

As the temperature of the host and surrounding geological formations increases, the heated materials will thermally expand.

Integrating the computed thermal deformations along a vertical up to the surface allows assessing the vertical displacement, or uplift, of the ground above the disposal system.

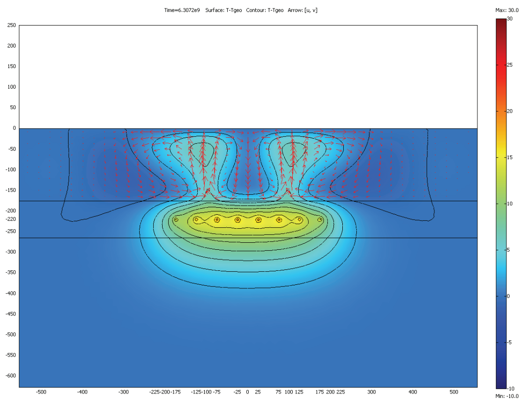

Figure 8. Temperature increase field ΔT, 200 years after the disposal of VHLW. The heat released from the clay is carried away by convection cells in the aquifer, which can develop in the absence of natural gradient.

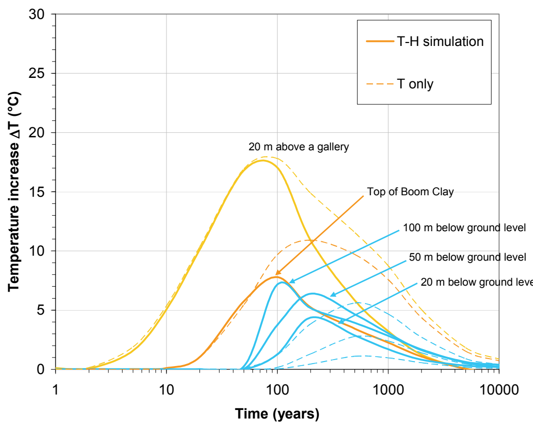

Figure 9. Time histories of temperature increase ΔT at various distances above the third gallery of the repository if convection cells develop. The temperature of the aquifer increases locally by 7.5°C.

When heated, both the solid and liquid phases of the porous media undergo thermal expansion. In high permeability layers, such as the Neogene aquifer, the excess water volume can quickly be accommodated through small water movements. In the low permeability Boom Clay, however, the thermal expansion of pore water results in overpressures in the pores. This, in turn, reduces the effective stresses of the clay, as the pore water temporarily bears an increased fraction of the total load on the porous media. Hence, in addition to the thermal expansion of its solid phase, the clay will undergo an additional deformation resulting from the decrease of the effective stresses. Typical thermal expansion coefficients for Boom Clay and the Neogene aquifer are summarized in Table 5.1, along with the thermal expansion coefficient of water.

Table 3: Typical thermal expansion coefficients

Material	Expansion coeff. (m^3/m^3 °C^{-1})	Symbol
Clay, drained	3×10^{-5}	β_d
Clay, undrained	13×10^{-5}	β_u
Water	21×10^{-5}	β_w
Sand, drained	3×10^{-5}	β_d

3.1 Model and data

Picard and Giraud [7] developed an analytical solution to the coupled thermo-hydro-mechanical problem defined by the heating of a homogeneous, isotropic horizontal layer of clay. In this one-dimensional vertical model, the medium is assumed to have a linear thermo-poro-elastic behaviour and the heat source is homogeneously spread horizontally. Under those assumptions, the system of partial differential equations describing the evolution in time and space of temperatures T, pore pressures p and the resulting deformations ε_z can be summarised as follows:

$$\frac{\partial T}{\partial t} = \alpha_T \frac{\partial^2 T}{\partial z^2} + \frac{q}{\lambda} \tag{9}$$

$$\frac{\partial p}{\partial t} = \alpha_H \frac{\partial^2 p}{\partial z^2} + \Lambda \frac{\partial T}{\partial t} \tag{10}$$

$$\varepsilon_z = \frac{p + \beta_d K_d T}{\lambda_d + 2G} \tag{11}$$

where z is the vertical coordinate, q is the heat source density, λ is the thermal conductivity of the saturated porous medium, α_T and α_H are the thermal diffusivity and hydraulic diffusivity respectively, K_d and G are the drained bulk modulus and the shear modulus of the porous medium, $\lambda_d = K_d - 2G/3$ is the drained Lamé coefficient and Λ is defined by

$$\Lambda = \left(\frac{\partial p}{\partial T}\right)_{undrained, oedometer} \tag{12}$$

For Boom Clay, the values of these parameters are given in Table 4.

Table 4: Boom Clay parameters (adapted from Picard and Giraud, 1995)

Parameter	Value	Units
α_T	7×10^{-8}	m^2/s
α_H	6×10^{-7}	m^2/s
λ	1.35	W/m/°C
Λ	18700	Pa/°C
K_d	100	MPa
G	60	MPa
K_u	5600	MPa

To compute the uplift, the diffusion problem defined by equations (9) and (10) is solved first then equation (11) is used to compute the deformations, which are in turn integrated along the vertical to obtain the displacements.

In the model of Picard and Giraud, the clay layer extends up to the surface and the system (9)-(10) can be easily diagonalized and solved analytically. However, this does not accurately represent the drained thermal expansion of the aquifer and the dissipation of the pore pressures from the Boom Clay into the aquifers. For this study, the model was updated with the inclusion of the aquifers above and below the Boom Clay and equations (9)-(11) are instead solved numerically using COMSOL Multiphysics.

3.2 Results

The evolutions of the vertical displacement of the ground (uplift) and the vertical displacements of the repository structure and of the limits of the Boom Clay are shown in Figure 10. The maximum computed uplift amounts to about 15 cm and should occur about 60 years after the disposal of the vitrified waste. The thermal expansion of the various layers can be obtained by taking the difference of the vertical displacement of the interfaces. Clearly, most of the uplift can be attributed to the Boom Clay.

4. Conclusions

In the context of a R&D programme on geological disposal of heat-emitting radioactive waste, Comsol Multiphysics was found to be a tool versatile enough to be used for the full scale simulation of the long-term evolution of a deep repository, in addition to its regular use in support of small-scale, experiment-based phenomenological analysis within the programme. The availability of a common modelling tool to phenomenology-minded scientists and system-oriented engineers working on a common, multi-disciplinary project is a significant asset.

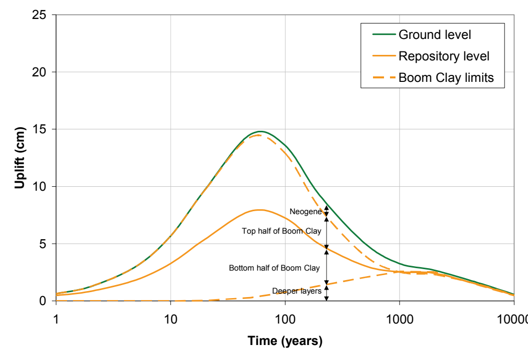

Figure 10. Evolutions of the vertical displacements.

5. References

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6. Acknowledgements

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