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# MODELING OF THE GROUNDWATER TRANSPORT AROUND A DEEP BOREHOLE NUCLEAR WASTE REPOSITORY

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## ABSTRACT

The concept of disposal of high-level nuclear waste in deep boreholes drilled into crystalline bedrock is gaining renewed interest and consideration as a viable mined repository alternative. A large amount of work on conceptual borehole design and preliminary performance assessment has been performed by researchers at MIT, Sandia National Laboratories, SKB (Sweden), and others. Much of this work relied on analytical derivations or, in a few cases, on weakly coupled models of heat, water, and radionuclide transport in the rock. Detailed numerical models are necessary to account for the large heterogeneity of properties (e.g., permeability and salinity vs. depth, diffusion coefficients, etc.) that would be observed at potential borehole disposal sites.

A derivation of the FALCON code (Fracturing And Liquid CONvection) was used for the thermal-hydrologic modeling. This code solves the transport equations in porous media in a fully coupled way. The application leverages the flexibility and strengths of the MOOSE framework, developed by Idaho National Laboratory. The current version simulates heat, fluid, and chemical species transport in a fully coupled way allowing the rigorous evaluation of candidate repository site performance.

This paper mostly focuses on the modeling of a deep borehole repository under realistic conditions, including modeling of a finite array of boreholes surrounded by undisturbed rock. The decay heat generated by the canisters diffuses into the host rock. Water heating can potentially lead to convection on the scale of thousands of years after the emplacement of the fuel. This convection is tightly coupled to the transport of the dissolved salt, which can suppress convection and reduce the release of the radioactive materials to the aquifer. The purpose of this work has been to evaluate the importance of the borehole array spacing and find the conditions under which convective transport can be ruled out as a radionuclide transport mechanism.

Preliminary results show that modeling of the borehole array, including the surrounding rock, predicts convective flow in the system with physical velocities of the order of  $10^{-5}$  km/yr over  $10^5$  years. This results in an escape length on the order of kilometers, which is comparable to the repository depth. However, a correct account of the salinity effects reduces convection velocity and escape length of the radionuclides from the repository.

## 1. INTRODUCTION

The final disposal of high-level spent nuclear fuel is an ongoing research topic. To date, no country has an operational licensed high-level waste disposal system.

In recent years, the issue of nuclear waste disposal has become one of the most controversial aspects of nuclear technology. After Yucca Mountain was closed down, 66,000 MTHM of spent nuclear fuel has been accumulated at interim storages in the United States [1]. The expansion of the nuclear industry in the United States depends on the development of a safe and socially acceptable permanent disposal method.

One of the proposed ideas is the entombment of the spent fuel in a borehole drilled into a crystalline basement rock. The spent fuel is put inside canisters which are emplaced into the deep boreholes. The boreholes are sealed with concrete and bentonite. This method of disposal relies on the geological properties of the rock rather than the canister integrity. The sites with suitable crystalline granite starting at most at 2 km depth are widely available in the US. In addition, a deep borehole repository can be cheaper than conventional mined repositories because of all the breakthroughs achieved in the oil drilling industry.

Regulations require the analysis of performance of the repository for a million years. Because of the complex processes to be analyzed, and the time and length scales involved in the problem, it is crucial to have an adequate modeling tool. This application should be capable of modeling accurately the thermal field and water flow around the borehole repository on different time and length scales. This requires a robust finite element code with strong coupling of all physical phenomena. An example of such a code is MOOSE (Multiphysics Object Oriented Simulation Environment) [2].

## 2. GOVERNING EQUATIONS

### 2.1 Thermal Model

Consider a control volume of rock. Then for the rock the heat balance equation can be written as

$$(1 - \varepsilon)\rho_r c_r \frac{\partial T_r}{\partial t} = (1 - \varepsilon)\nabla \cdot (k_r \nabla T_r) + (1 - \varepsilon)q''', \quad (1)$$

and for the fluid

$$\varepsilon\rho_f c_f \frac{\partial T_f}{\partial t} + (\rho_f c_f) \vec{j} \nabla T_f = \varepsilon \nabla \cdot (k_f \nabla T_f), \quad (2)$$

where the subscripts  $r$  and  $f$  refer to the rock and water, respectively,  $c$  is the specific heat of the material,  $k$  is the thermal conductivity,  $\vec{j}$  is the superficial velocity,  $q'''$  is the heat generation per unit volume, and  $\varepsilon$  is porosity.

Assume that rock and water are in equilibrium so that  $T_r = T_f = T$ . Summing Eqs. (1) and (2) and considering that porosity is very small one can obtain:

$$\rho_r c_r \frac{\partial T}{\partial t} + (\rho_f c_f) \vec{j} \nabla T = \nabla \cdot (k_r \nabla T) + q'''. \quad (3)$$

### 2.2 Fluid Model

The equations that control the dynamics are the continuity equation and Darcy's law:

$$\frac{\partial(\epsilon\rho_f)}{\partial t} + \nabla(\rho_f \vec{j}) = 0, \quad (4)$$

$$\nabla P - \rho_f \vec{g} + \frac{\mu}{K} \vec{j} = 0, \quad (5)$$

where  $P$  is pressure,  $K$  is the host rock permeability,  $\mu$  is the water dynamic viscosity, and  $\vec{j}$  is the Darcy (superficial) velocity. The real physical velocity of the water is related to the superficial velocity as

$$\vec{v} = \frac{\vec{j}}{\epsilon} \quad (6)$$

Eqs. (4) and (5) can be combined together:

$$\frac{\partial(\epsilon\rho_f)}{\partial t} + \nabla\left(\frac{K\rho_f}{\mu}(\rho_f \vec{g} - \nabla P)\right) = 0. \quad (7)$$

Water viscosity and density are functions of pressure and temperature. In this work water properties are taken from IAPWS-97 steam tables.

Taking into account that  $\frac{\partial\rho_f}{\partial P} = \beta_p \rho_f$ , where  $\beta_p$  is the compressibility of water, Eq. (7) becomes a diffusion equation for pressure with a pressure diffusivity  $\alpha_p = K / \mu \beta_p \epsilon$ . This value is used later to explain water flow behaviour at different time and length scales.

### 3. NUMERICAL IMPLEMENTATION

MOOSE framework [2] was used to solve this problem. This framework was designed to simplify development of fully-coupled, parallel, fully implicit, nonlinear finite element applications. MOOSE is based on the mathematical principle of the Jacobian-free Newton-Krylov method, although it also has a Newton solver. MOOSE requires only residual evaluations of the discretized equations, which allows modularization of all equations into so-called “kernels”.

FALCON (Fracturing And Liquid CONvection) is an application developed in MOOSE for modelling of the fluid flow, heat transport, and rock deformation in enhanced geothermal systems [3]. Eqs. (3) and (7) are implemented in FALCON along with other equations.

A number of modifications were made to FALCON in order to model the deep borehole repository. First, the temperatures in the rock around the borehole never exceed saturation pressure at the given pressure. No fast flow of water that may cause water boiling is expected. For this reason fluid model was reduced to a single phase pressure-temperature formulation.

Secondly, the kernels for salinity transport were implemented into the code. They include salinity diffusion, time derivative term, and advection term with isotropic SUPG term to make the code stable. Also, this addition lead to modifications to the water equation of state.

All runs were performed in two steps. First, a steady problem was solved to achieve a steady state of pressure and temperature without heat generation in the canisters. After that a transient simulation was run using the output of the first step as an initial condition.

#### 4. PROBLEM PARAMETERS

The performance of the deep borehole repository depends on many properties of both rock and repository. It should be noted that neither a place for a repository nor final design of the boreholes and canisters is selected. For the purpose of the current research many parameters were taken from the reference models developed at MIT [4, 1, 5].

There is a number of site-specific parameters like rock permeability, chemical composition of the rock, density, thermal conductivity, and geothermal flux. These parameters may vary over a wide range. However, for a deep borehole repository certain properties are more favorable. For example, regions with lower geothermal flux are less susceptible to convection of the water and less attractive to possible use of these regions as sources of geothermal energy. Regions with very high rock permeability may have very strong convection while regions with very low permeability may have very high overpressure due to water expansion, resulting in cracks in the rock.

An overview of the rock permeabilities is given in [6]. Most of the experiments give permeability in the range  $10^{-17}$ – $10^{-14}$  m<sup>2</sup>. In this paper  $10^{-16}$  m<sup>2</sup> was assumed as a reference permeability. The rock porosity was assumed to be 1%.

An overview of salinity experiments was performed at MIT [7]. A polynomial dependence of salinity on depth was chosen for the current study:

$$\begin{aligned} S &= 1.234 \times 10^{-4} z^2 - 5.9419 \times 10^{-2} z + 5.8446, \\ S_{\max} &= 350 \text{ g/L}, \end{aligned} \quad (8)$$

where  $z$  is in meters and  $S$  is in g/L. For the equation of state the following correlation was used:

$$\rho_{\text{brine}} = 0.795S + \rho_{\text{ref}}, \quad (9)$$

where  $\rho_{\text{ref}}$  is the table value of fresh water density at the given pressure and temperature, and  $\rho_{\text{brine}}$  is the density of the brine.

The parameters of the repository include borehole diameter, emplacement depth, pitch length, fuel burnup, and interim storage time.

The decay heat was taken from [5] for 25 year-cooled, 57 MW-d/kg PWR spent fuel:

$$q''(t) = 2176 \left( \frac{t_c}{t_c + t} \right)^{0.75} \text{ W/m}^3. \quad (10)$$

The heat source is distributed uniformly in a homogenized canister with diameter of 34 cm. All other properties like the specific heat and thermal conductivity are also homogenized across the canister. Both canister and borehole seal are assumed to be permeable to water with the same permeability and porosity as the rock.

Typical values of the site and repository properties are summarized in Tables 1 and 2, respectively.



Table 1. Summary of site properties.

Parameter	Value
Rock density	2750 kg/m <sup>3</sup>
Thermal conductivity of rock	3 W/(m·K)
Specific heat of rock	790 J/(kg·K)
Geothermal flux	45 mW/m <sup>2</sup>
Temperature gradient	15 K/km
Surface temperature	10 °C (283 K)
Porosity	0.01 (1%)
Rock permeability	10 <sup>-16</sup> m <sup>2</sup>
Thermal diffusivity	1.38×10 <sup>-6</sup> m <sup>2</sup> /s

Table 2. Summary of the repository properties.

Parameter	Value
Borehole spacing	200 m
Borehole diameter	0.34 m
Emplacement region depth	3 to 5 km
Fuel burnup	57 MW-d/kg
Interim storage time	25 years
Average thermal conductivity of canister	0.628 W/(m·K)
Average specific heat of canister	499 J/(kg·K)

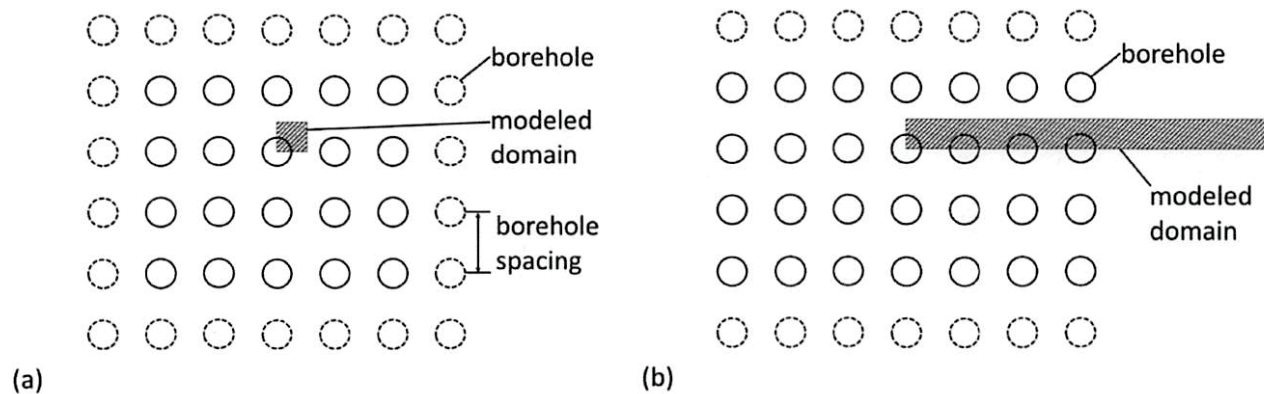


Figure 1. Regions being modeled (a) in the infinite array and (b) the semiinfinite array, not to scale.

## 5. INFINITE ARRAY

The simplest approach to the modeling of the deep borehole repository is to consider an infinite array of boreholes arranged in a square lattice with fresh water underground. Due to the symmetry this arrangement can be modeled on a domain containing one quarter of one borehole (Fig. 1(a)). All vertical boundaries are symmetry planes with Neumann boundary conditions for all variables. The bottom boundary is set deep enough so that it does not affect the solution. It was set at the depth of 10 km which is also a realistic estimate of the depth where brittle to ductile transition in rock occurs [1].

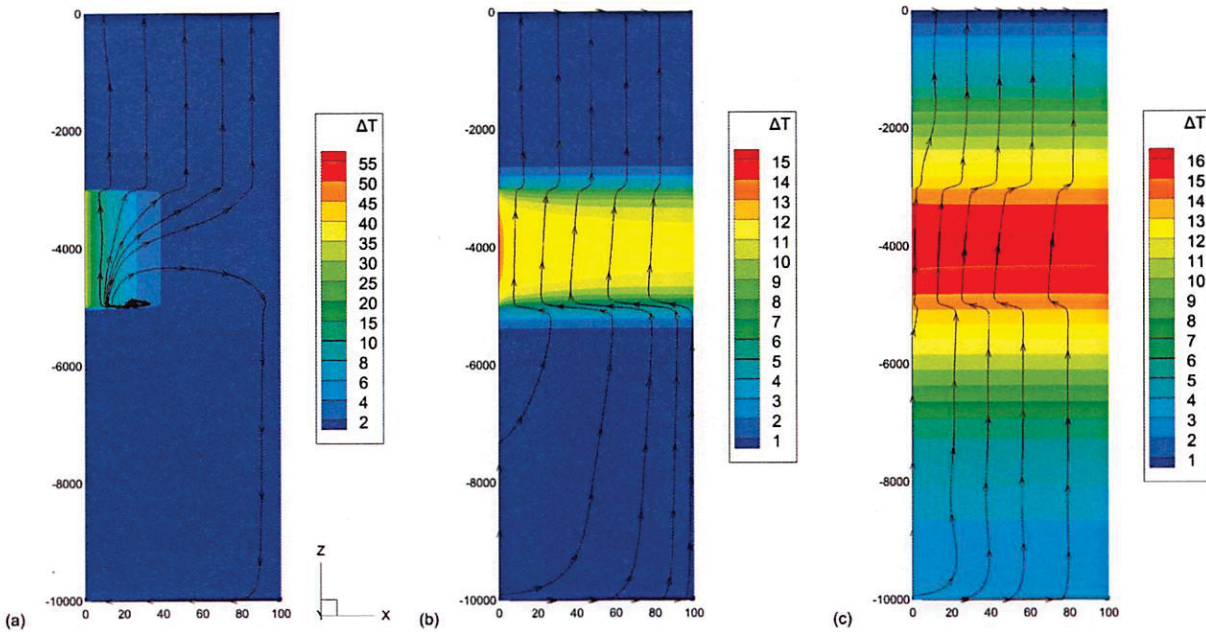


Figure 2. Temperature increase due to decay heat and streamlines around one borehole in the infinite array (not to scale): (a) 10 years after emplacement, (b) 1,000 years after emplacement, (c) 100,000 years after emplacement.

The results of the modeling are shown in Fig. 2 for 10, 1,000, and 100,000 years after the fuel entombment. The figure shows streamlines and temperature change due to emplaced nuclear fuel. For plotting purposes all plots are stretched in the horizontal direction by the factor of 30 (the aspect ratio of the region modeled is 1:100).

In Fig 2(a) (10 years after the fuel emplacement) the heat wave starts to propagate from the borehole, but most of the rock remains at the initial temperature. Later in time the heat wave reaches the symmetry boundary between adjacent boreholes. As a result, the emplacement region becomes uniformly heated (Fig. 2(b)) and the heat diffuses in the vertical direction.

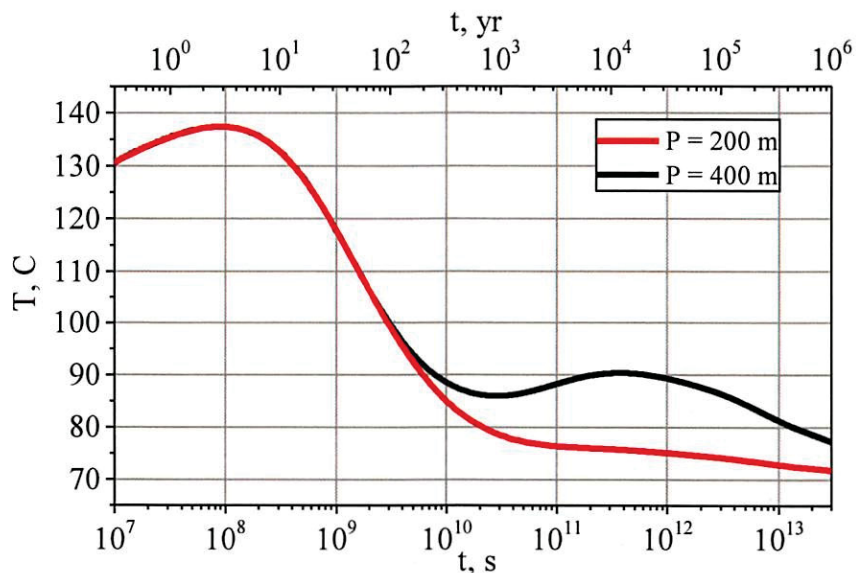


Figure 3. Centerline temperature in the fuel at the depth of 4 km as function of time for different borehole spacing.



A typical dependence of the fuel temperature on time is shown in Fig. 3. The maximum temperature is reached at about 5 years after the fuel emplacement. After this peak the centerline temperature decreases due to decrease of the decay heat. However, when the heat wave reaches the symmetry boundary, the temperature rises again. For a borehole spacing of 200 m or smaller a second peak in temperature can be seen. This peak temperature might be a limiting factor for the choice of borehole spacing [2, 3].

Fig. 2 shows that the streamlines above the borehole (in the caprock) are vertical. There is a certain level of convection in the emplacement zone, but in the caprock zone the flow is uniform. The vertical components of the superficial and physical velocities for different rock permeabilities and pitch lengths are shown in Fig. 4. The velocities behave in a very similar way at 1,000 years and later for fixed pitch length.

Define an escape length as

$$L = \int v dt. \quad (11)$$

For all the cases the escape length does not exceed 30 m. This means that groundwater flow cannot transport radionuclides further than 30 m through the caprock.

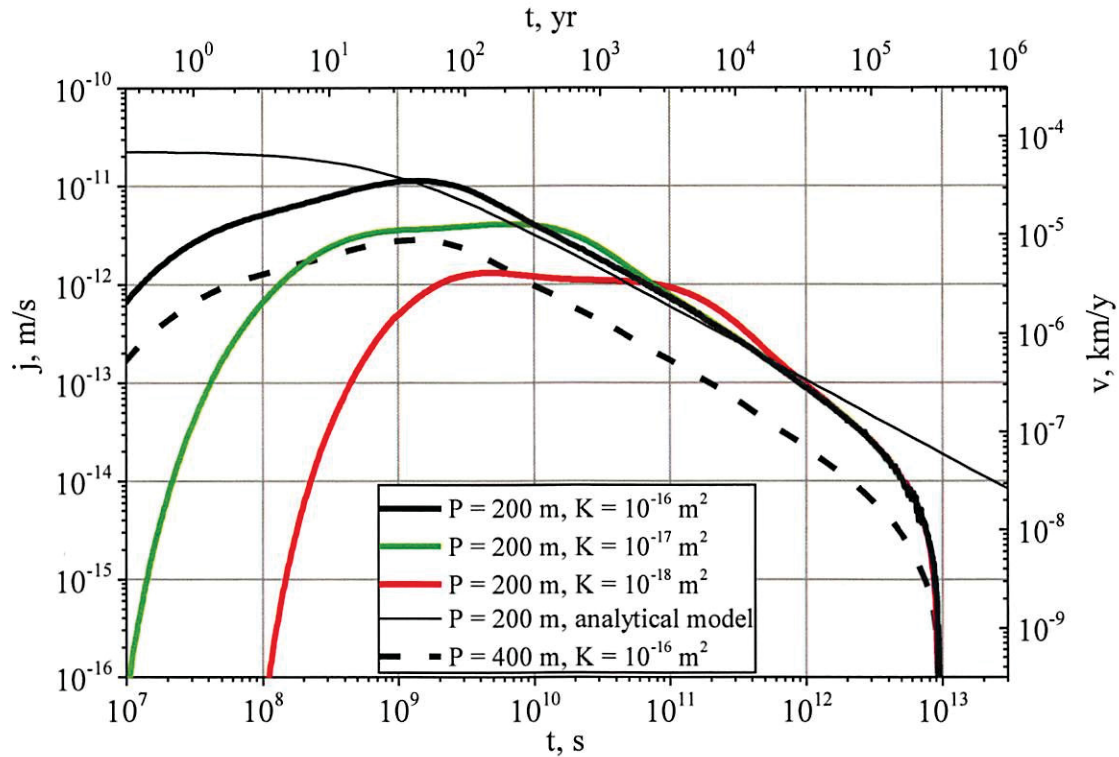


Figure 4. Vertical component of the groundwater velocity above the borehole at the depth of 2 km for an infinite array of boreholes.

### 5.1 Analytical model

The results show that the flow in the caprock at 100 years – 10,000 years is proportional to heat generation. This observation can be explained with a simple model. The heat diffusivity in the rock is  $\alpha_T = k/\rho c = 1.38 \times 10^{-6} \text{ m}^2/\text{s}$ , while the pressure diffusivity is  $\alpha_p = K/\mu\beta_p\varepsilon \approx 5 \times 10^{-2} \text{ m}^2/\text{s}$ . This means that at the given timescale and a length scale of 1,000 m pressure diffusion almost reaches steady state, while the heat wave from the borehole has not reached the end of the domain.



Assume that all properties, including those of water, do not depend on temperature and pressure. The averaged value of the water thermal expansion coefficient is taken at  $5 \times 10^{-4} \text{ K}^{-1}$ . Consider a region of the rock around one borehole below 2 km. The heat is produced at a rate

$$P(t) = q'''(t) \cdot V_{fuel} = q'''(t) \cdot L_{emplacement} \cdot \pi r^2 \quad (12)$$

Define the average temperature of the rock as

$$T_{av} = \frac{\int T dV}{V_{rock}} \quad (13)$$

Then the rate of change of the average temperature is

$$\frac{dT_{av}}{dt} = \frac{q'''(t) \cdot L_{emplacement} \pi r^2}{\rho_{rock} c_{p,rock} V_{rock}} \quad (14)$$

The region contains a volume of water  $\varepsilon V_{rock}$ . The expansion of water due to the heat generation is

$$dV = \beta_T \varepsilon V_{rock} dT_{av} \quad (15)$$

This extra volume of the water can leave the domain only through top surface. Therefore, the superficial velocity can be computed as

$$j(t) = \frac{dV}{A \cdot dt} = \frac{\varepsilon \beta_T L_{emplacement} \pi r^2 \cdot q'''(t)}{A \rho_{rock} c_{p,rock}}, \quad (16)$$

where  $A$  is the area per borehole in the infinite array.

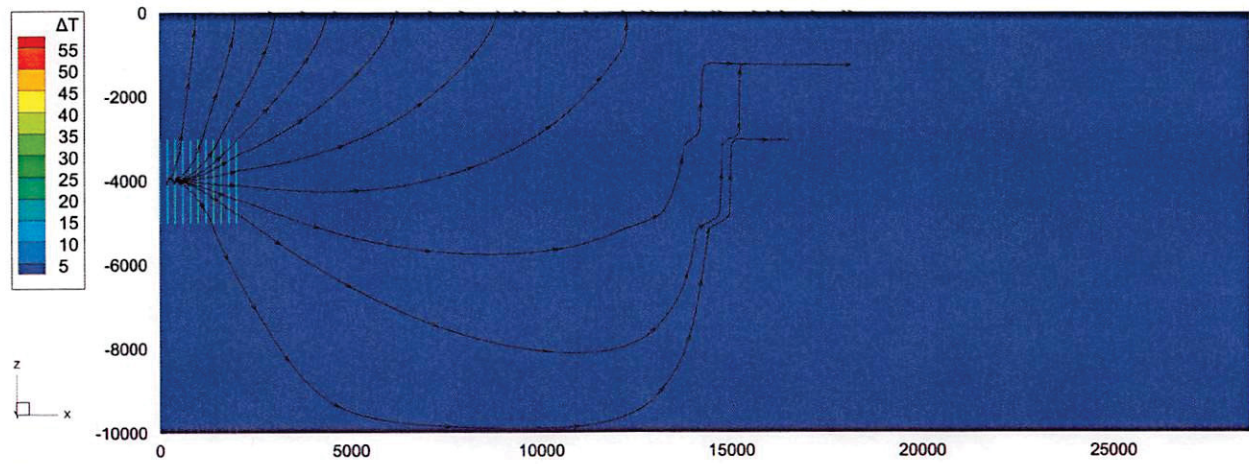
The analytical solution is shown in Fig. 4 along with the numerical results obtained with FALCON. In the first 100 years velocity derived from the simplified model differs from the numerical results. This is due to the response time required for a pressure wave to travel to the region where velocity is monitored. The response time increases with the decrease of permeability, so for lower  $K$  the region where the model works is narrower. 300,000 years after fuel emplacement the modeled superficial velocities become negative. This is due to diffusion of heat outside of the domain, which reduces the average temperature of the domain and causes water to flow back. At this moment the model fails to predict the correct groundwater flow, but remains conservative.

## 6. SEMIINFINITE ARRAY

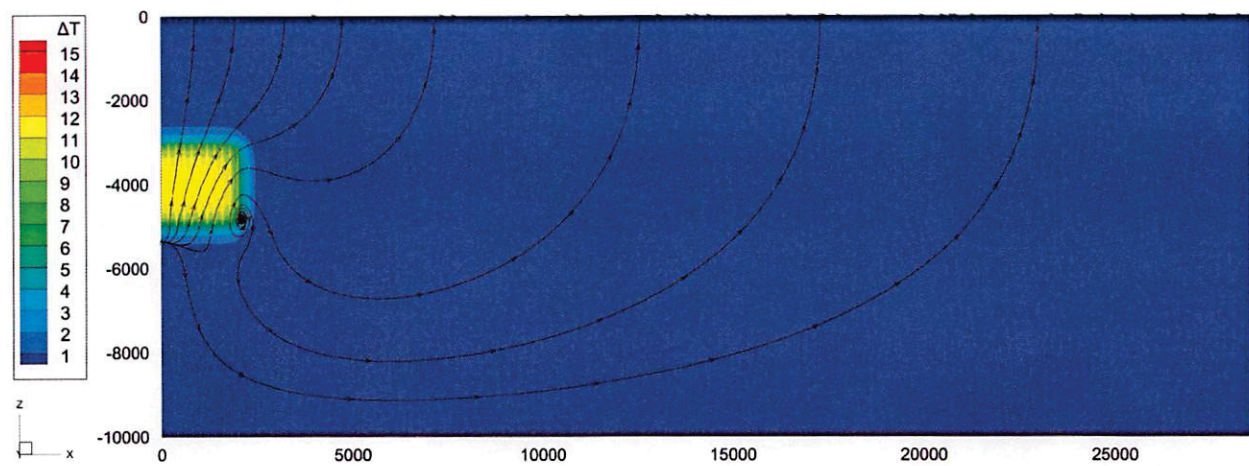
The infinite model assumed that the array of boreholes is large enough to consider the central region behavior independent of the boundary condition. It was assumed that the flow in this region is the highest and that it is limiting for the performance of the whole repository. However, this approach misses the phenomena occurring at the boundary between the array of boreholes and undisturbed rock.

Modeling of the complete site with more than 500 boreholes is challenging from a numerical point of view due to memory and computational power limitations. To get round this limitation a semiinfinite model was proposed (Fig. 1(a)). In this model the boreholes are assumed to be arranged in an infinite line of constant number of boreholes in width. This allows one to keep the physical model close to realistic with a relatively small domain due to symmetry of the model. The width of the full site was taken to be

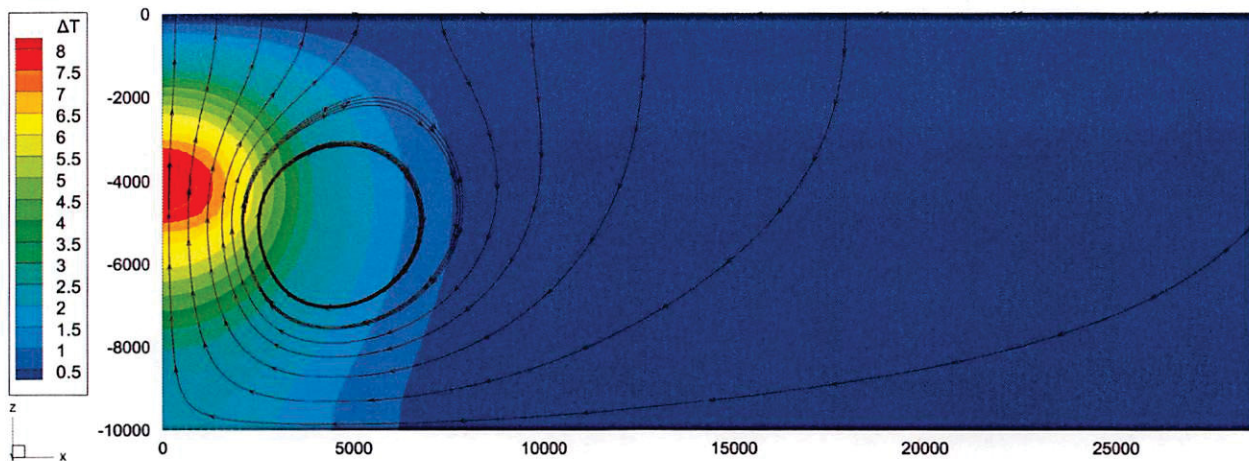
21 boreholes, so 10 half-boreholes and one quarter-borehole were included in the mesh. The outer boundary was set at 40 km away from the repository to minimize its effect on the flow inside the repository.



(a)



(b)



(c)



Figure 5. Temperature increase due to conduction of decay heat, and streamlines in the semiinfinite array: (a) 10 years after emplacement, (b) 1,000 years after emplacement, (c) 100,000 years after emplacement.

The results of the modeling are shown in Fig. 5 for 10, 1,000, and 100,000 years after the fuel entombment. As for the infinite array the temperature change was used for coloring. The repository is located at the left (see the vertical lines in Fig. 5(a)).

The results are different from the infinite array case. At 10 and 1,000 years after fuel emplacement water flow is directed away from the repository and is caused by water expansion. However, at 100,000 years the borehole site is uniformly heated and a clear convective loop is created through the repository.

The vertical components of the velocities at the center of the repository are shown in Fig. 6. One can see that at 1–1,000 years the velocity is even smaller than in the infinite array case since there are more paths available for the water to escape. However, at 1,000 years after the fuel entombment the velocity does not decrease proportionally to the decay power  $q'''(t)$ . Instead it creates a second peak at 50,000 years.

Convection in the semiinfinite array might be troubling for the performance of the repository. A physical velocity of  $10^{-5}$  km/yr for  $10^5$  years leads to the escape length of the order of kilometers, which is comparable to the disposal depth. For example, the escape length at 250,000 years for rock permeability of  $10^{-16}$  m<sup>2</sup> and  $10^{-17}$  m<sup>2</sup> is 2390 m and 987 m, respectively. Such flow can potentially transport radionuclides from the repository to a near-surface aquifer.

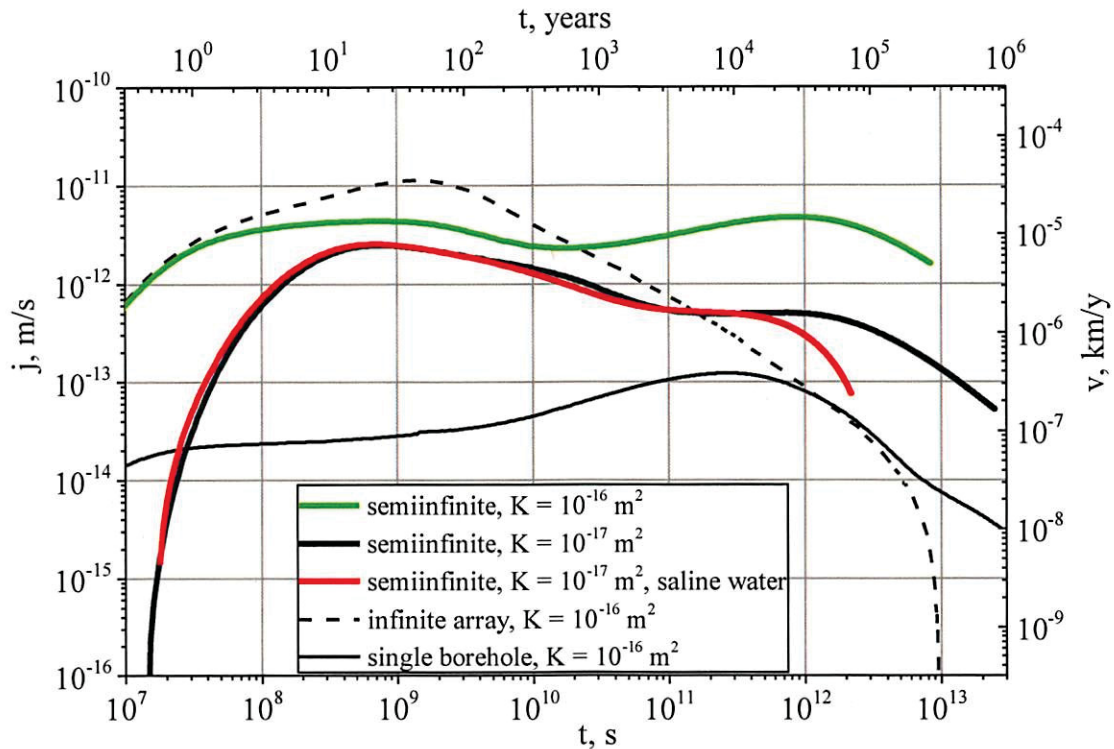


Figure 6. Vertical component of the groundwater velocity above the borehole at the depth of 2 km for the semiinfinite array of boreholes.

## 6.1 Effect of salinity on convection

An important assumption made was that underground water is fresh. However, in reality water salinity increases with depth, reaching some constant saturated value [4]. If the water moves upward above the borehole the salinity front is also moved upward. This creates an additional hydrostatic pressure which suppresses convection.

Results including salinity transport are shown in Fig. 6 with a red line. Due to the numerical complexity of the code we were unable to reach time larger than 70,000 years for rock permeability of  $10^{-17} \text{ m}^2$ . However, even at this time the addition of salinity reduces the velocity almost by a factor of 10. The sample profile of salinity above the borehole repository is shown in Fig. 7. Salinity difference at this depth creates a hydrostatic gradient difference of around  $3 \text{ g/L} \times 9.81 \text{ m/s}^2 = 30 \text{ Pa/m}$  over around 1000 m of the region of high salinity gradient, which is comparable to the pressure driving convection and causes significant reduction of the velocity.

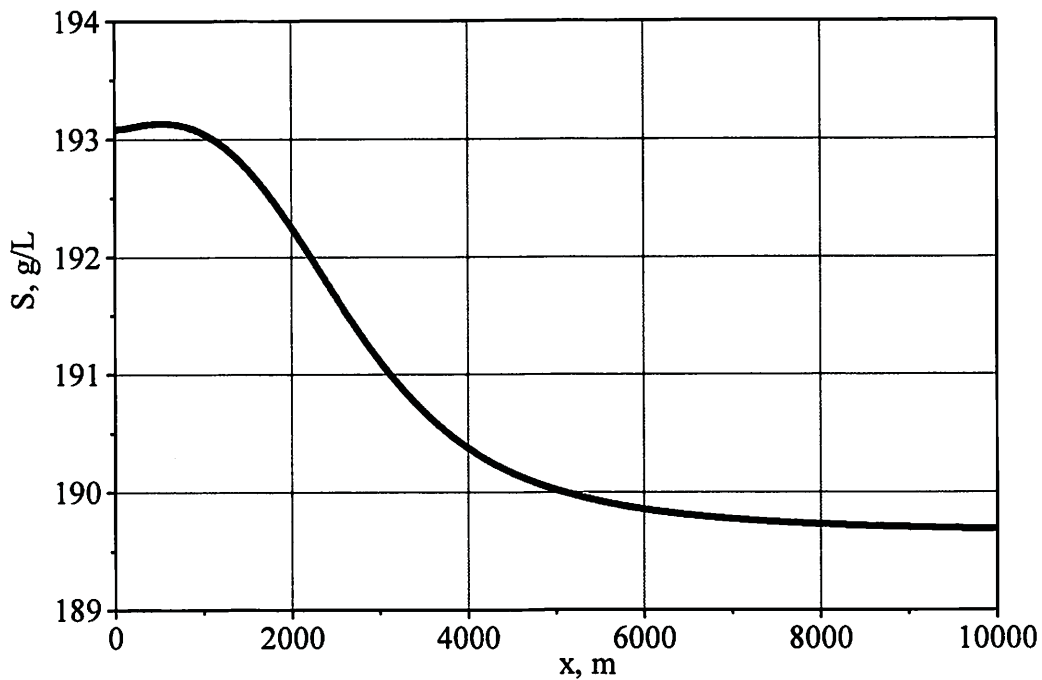


Figure 7. Salinity profile at the depth of 1500 m above the repository 70,000 years after fuel emplacement.

## 7. CONCLUSIONS

A fully coupled analysis of a complete repository is important for understanding of the processes around a deep boreholes repository. An infinite array model may seem conservative at first sight but it underestimates the groundwater flow above the repository since it cannot capture all physical phenomena. Repository modelling including the surrounding rock allows producing more realistic results, but is also challenges the solution methods of the code and requires considerably higher computational requirements.

Future investigation will be focused on the improvement of the code robustness and addition of a more complete description of all relevant physical phenomena, including but not limited to chemical transport and rock deformation.



## 8. ACKNOWLEDGEMENTS

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