

Thermal Response of a Mark II Conceptual Deep Geological Repository in Crystalline Rock

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ABSTRACT

Title: Thermal Response of a Mark II Conceptual Deep Geological Repository in Crystalline Rock
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Abstract

This report describes the thermal performance of a conceptual deep geological repository (DGR) involving the Mark II container and placement concept in a hypothetical crystalline rock environment.

A series of design studies for conceptual DGRs has been carried out over the past 30 years. These studies include two- and three-dimensional thermal transient and thermo-mechanical analyses. For numerical reasons, they are divided into far-field modelling and near-field modelling. In the Near-Field Models, an adiabatic thermal condition is applied on the four vertical outside boundaries, and as such, this represents a repository with an infinite horizontal dimension. The results from such models are known to be accurate at early times, with the thermal response overestimated at longer times.

To examine the influence of this boundary condition, thermal near-field modelling is performed for the Mark II repository using COMSOL and a method is proposed to account for boundary condition influences. The method is validated by comparing the modified COMSOL results with a theoretical solution produced using HOTROK.

A great portion of the temperature change at later times in the non-modified near-field modelling results is attributed to the effect of the adiabatic condition applied on the four vertical boundaries. The modified analysis shows that the thermal peak occurs early in the life of the repository and there is no comparable second peak after thousands of years for the case described in this report.

For the case evaluated, the maximum container surface temperature is 84°C occurring after 45 years, the maximum temperature of the room centre between two containers is 83°C occurring after 45 years, and the maximum temperature of the rock is 77°C occurring at the room roof above the top layer container after 65 years.

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1. INTRODUCTION

The Adaptive Phased Management (APM) approach for the long-term management of Canada's used nuclear fuel includes placement of the used fuel in engineered excavations around 500 m deep in either crystalline or sedimentary rock (NWMO 2005).

The used-fuel container corrosion rate, the performance of the sealing materials around the containers, and the mechanical stability of the surrounding rock around the placement rooms all depend on the thermal response in the repository. Thermal analyses is therefore important for repository design and for repository safety.

A series of conceptual design studies for a deep geological repository (DGR) has been carried out in the past (Acres et al. 1985, 1993; Mathers 1985; Tsui and Tsai 1985; Golder Associates Ltd. 1993; Baumgartner et al. 1994; Guo 2007, 2008). These studies include two- and three-dimensional thermal transient and thermo-mechanical analyses. For numerical reasons, the analyses are divided into near-field modelling and near-field modelling.

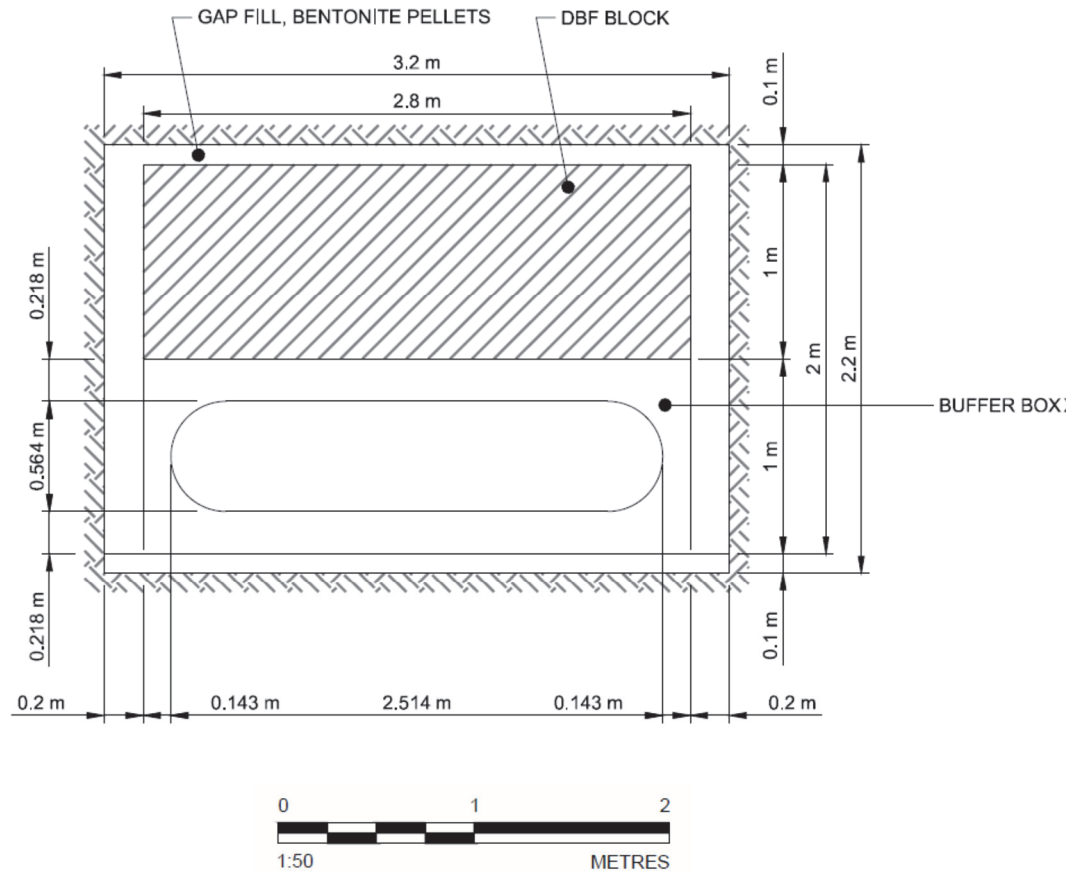
In these near-field models, an adiabatic thermal boundary condition is applied on the four vertical outside boundaries and as such, this represents a repository with an infinite horizontal dimension. For a finite dimension repository, results generated with this approach are accurate at early times and the thermal response is overestimated at longer times. To correct for this, Guo (2007) proposed a method for modifying near-field thermal results. This approach is further revised in this study and applied to the case of a conceptual Mark II repository in crystalline rock.

This report contains the following:

- A description of the modelled DGR scenarios.
- Material properties used in the models.
- Thermal near-field modelling.
- Thermal far-field modelling.
- Influences of the thermal boundary conditions used in the near-field model.
- Validation of the method proposed for modification of the near-field modelling results.
- Summary and conclusions.

2. DESCRIPTION OF A PROPOSED DEEP GEOLOGICAL REPOSITORY

The conceptual DGR layout to be modelled using COMSOL (COMSOL 2015) consists of an array of horizontal rectangular-shaped placement rooms (Figure 1). The placement room is 2.2 m high, 3.2 m wide and 308 m long.

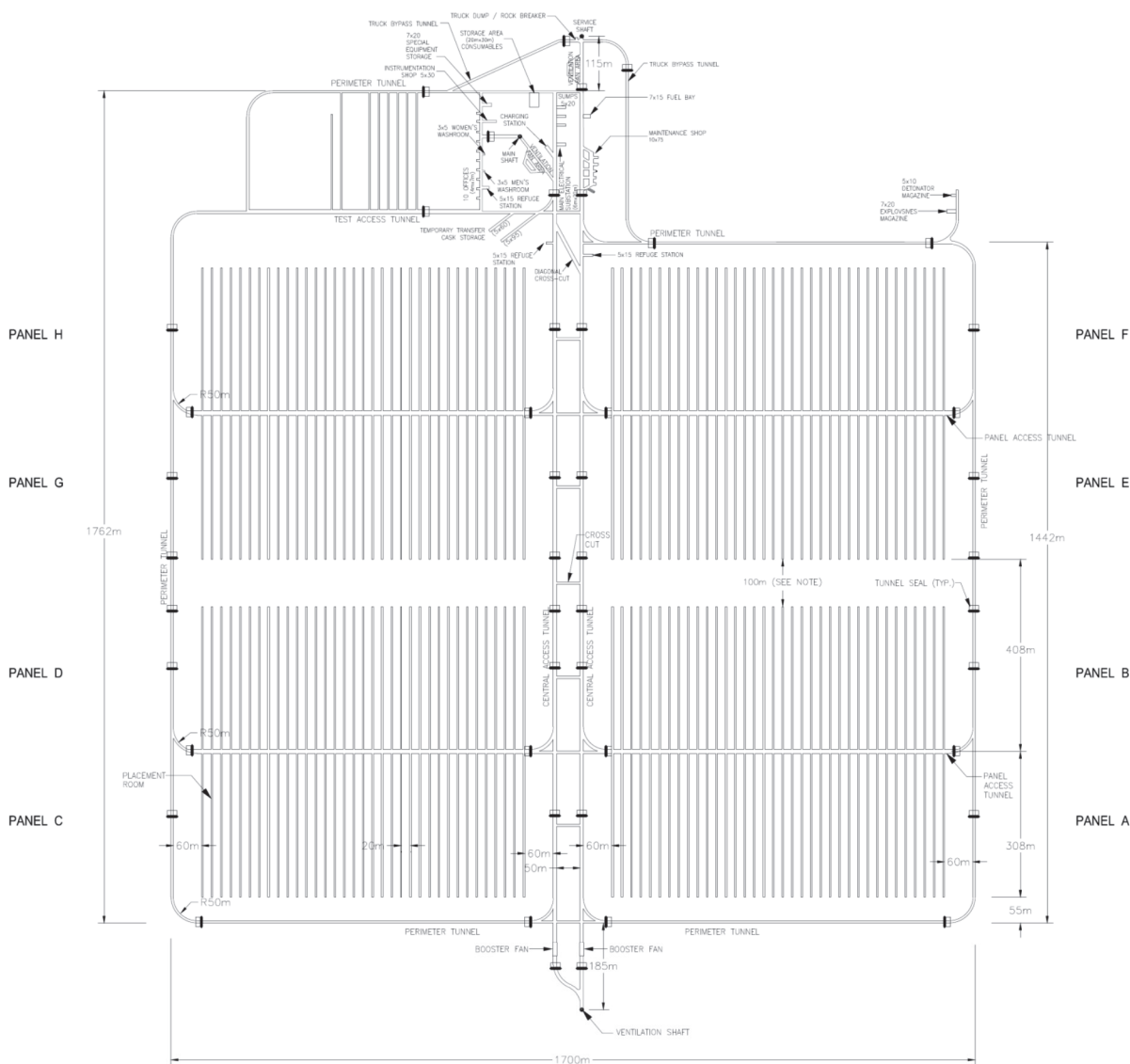


Source: APM-DRAW-22100-0001-R000 with Used Fuel Container (UFC) dimensions modified

Figure 1: Sectional View of Placement Room

Access tunnels connect the placement rooms for moving personnel, material, excavated rock, used-fuel storage containers and backfilling materials. These rooms are arranged into several distinct sections or panels. Each panel consists of a number of placement rooms (Figure 2), each room containing a number of Mark II used-fuel containers within two layers. One Mark II used-fuel container is horizontally placed in a bentonite box which is placed perpendicular to the tunnel axis (Figure 1). Between two bentonite boxes is a dense backfill block (Figure 3). Each Mark II container is 2.8 m long with a diameter of 0.564 m and accommodates 48 used CANDU® fuel bundles. The container design consists of a 3 mm-thick copper outer corrosion-barrier and an inner, carbon-steel load-bearing component. The conceptual DGR has a minimum total capacity of about 4.6 million intact fuel bundles or about 96,000 Mark II used-fuel

containers (UFCs). Dimensions of the repository, placement room, containers and sealing materials are shown in Figure 1 through Figure 3.

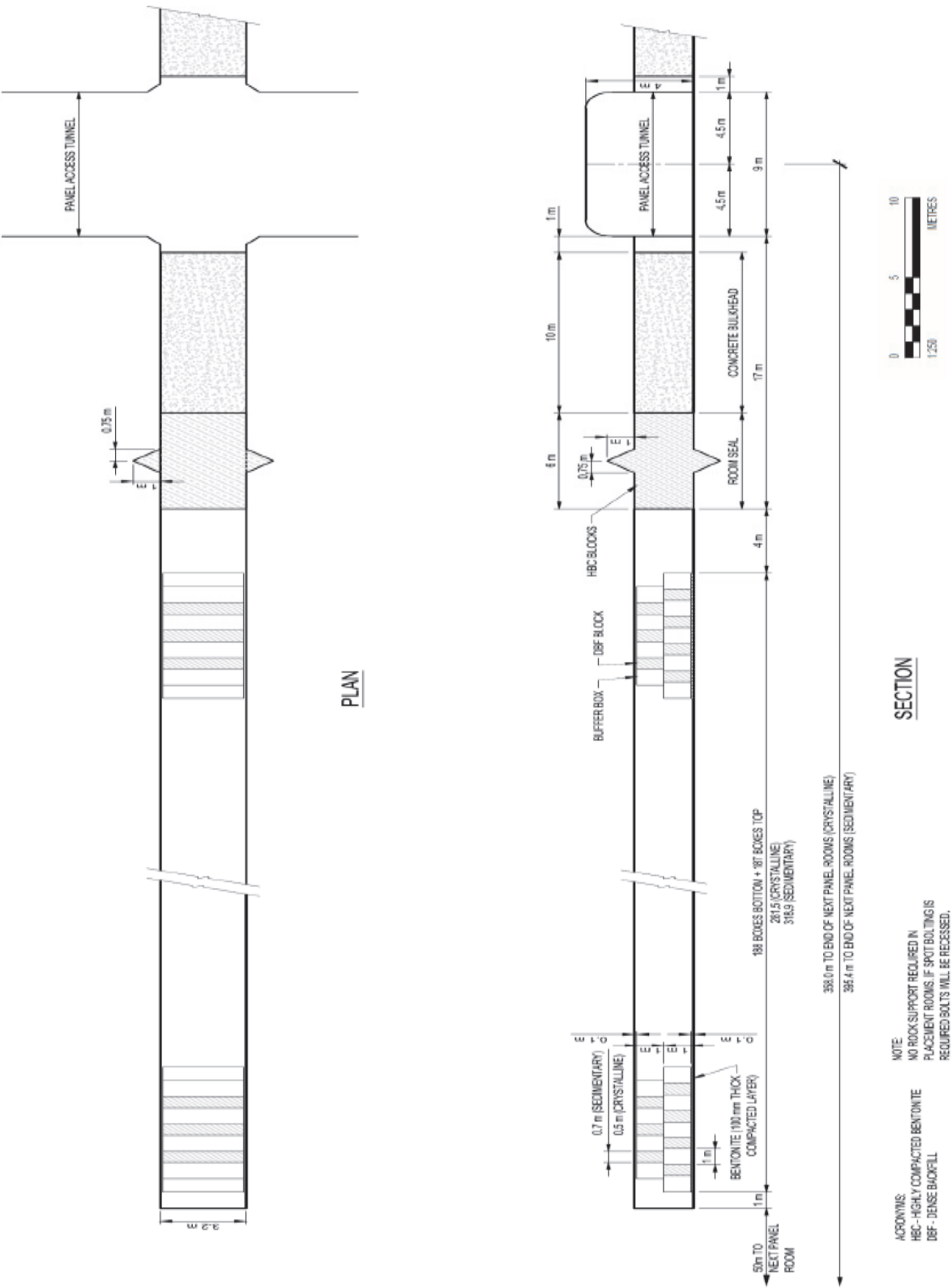


NOTE:

100m SEPARATION BETWEEN PANELS B/D AND PANELS E/G IS NOMINAL. NWMO MAY ADJUST SEPARATION TO ACCOMMODATE HYPOTHETICAL GEOLOGIC STRUCTURE THAT IS ASSUMED TO INTERSECT UNDERGROUND REPOSITORY AT THIS LOCATION.

Source: APM-GA-22100-0009-R000

Figure 2: Mark II Crystalline Underground Layout for 4.6 Million Bundles



Source: APM-DRAW-22110-0005-R000

Figure 3: Plan View and Longitudinal Section of Placement Room

3. ASSUMPTIONS AND MATERIAL PROPERTIES

3.1 ASSUMPTIONS

Each of the repository materials is assumed to be homogeneous and isotropic with temperature-independent properties. The rock mass around the DGR is assumed infinite in horizontal extent.

3.2 MATERIAL PROPERTIES

USED-FUEL PROPERTIES

The heat output from the used fuel in each storage container is shown in Table 1 (Tait et al., 2000). The fuel is assumed to have a burnup of 220 MWh/kgU and to undergo an initial cooling period of 30 years prior to placement. The DGR is assumed to be filled instantaneously with 30-year-out-of-reactor fuel at the reference conditions.

Table 1: Heat Output of a Container of Reference Used CANDU Fuel (220 MWh/kgU Burn-up) at Different Times

Time out-of-reactor (years)	Q per container (W/container) (48 bundles)	Time out-of-reactor (years)	Q per container (W/container) (48 bundles)
30	169.092	150	46.108
35	155.232	160	44.075
40	142.296	200	38.716
45	131.208	300	32.802
50	121.968	500	26.888
55	112.728	1000	18.665
60	105.336	2000	12.751
70	91.568	5000	9.240
75	85.932	10000	6.644
80	80.850	20000	3.844
90	72.257	35000	2.097
100	65.327	50000	1.321
110	59.783	100000	0.380
135	49.988	1000000	0.137

ROCK-MASS PROPERTIES

The material properties of the rock mass are based on measurements from Lac du Bonnet granite at the Underground Research Laboratory (Martin 1993) and are included in Table 2.

Table 2: Thermal Parameters for the Materials Considered in the Modelling

Property	Granite	Highly compacted bentonite	Gap fill (bentonite Pellets)	Dense backfill	Container
Thermal conductivity (W/m°C)	3.00	1.00	0.4	2.00	60.5
Specific heat (J/kg°C)	845	1280	870	1060	434
Bulk Density (kg/m ³)	2700	1955	1439	2276	7800

SEALING-MATERIAL AND USED-FUEL CONTAINER PROPERTIES

There are three bentonite clay-based sealing materials: buffer box material, dense backfill and buffer pellets. The buffer is placed around the container in the form of close-fitting, pre-compacted boxes with a saturation of 67%. The gaps between the buffer boxes/dense backfill blocks and the tunnel surface will be filled using a pelletized form of the buffer material with a saturation of 6%. The dense backfill has a saturation of 80%. Thermal properties for the clay-based sealing materials are determined using calculations illustrated in Baumgartner (2006) and shown in Table 2. (Note that effects of dry out on buffer properties are not included in this analysis.)

The thermal conductivity, the density and the specific heat of the used-fuel container are also shown in Table 2.

4. THE NEAR-FIELD MODEL

4.1 MODEL GEOMETRY AND THERMAL BOUNDARY CONDITIONS

4.1.1 Near-Field Model Geometry

The geometry of a unit cell for the Near-Field Model is shown in Figure 4. There are five kinds of materials: granite rock, dense backfill blocks, bentonite buffer boxes, container and bentonite pellets. The dimensions of the placement room are the same as shown in Figure 1. The horizontal dimensions of a unit cell are 10 m x 0.75 m (0.75 m is 1/2 of container spacing (from centre to centre) at the same layer, 10 m is 1/2 of placement-room spacing (from centre to centre)). The vertical dimension of the model unit cell is 10,000 m. The depth of the bottom of the placement room is 500 m.

Figure 4: Geometry for Near-Field Unit Cell

Tetrahedral elements are used through the model. The elements are more densely distributed in the region of high thermal gradients as shown in Figure 5 (near the placement room). There are a total of 97,092 tetrahedral elements.

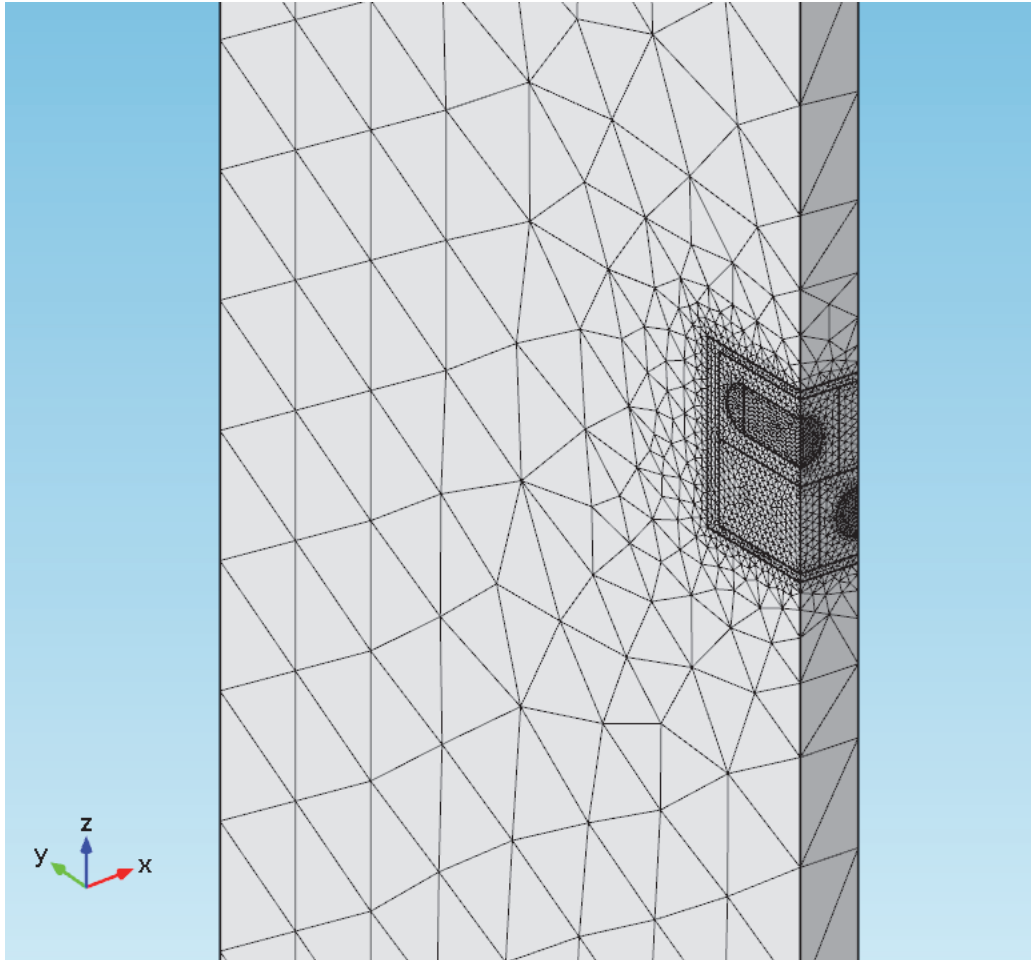


Figure 5: Finite Element Discretization of the Central Part of the Unit Cell for Near-Field Analyses

Figure 6 shows the locations at which the Near-Field Model results will be output in this report.

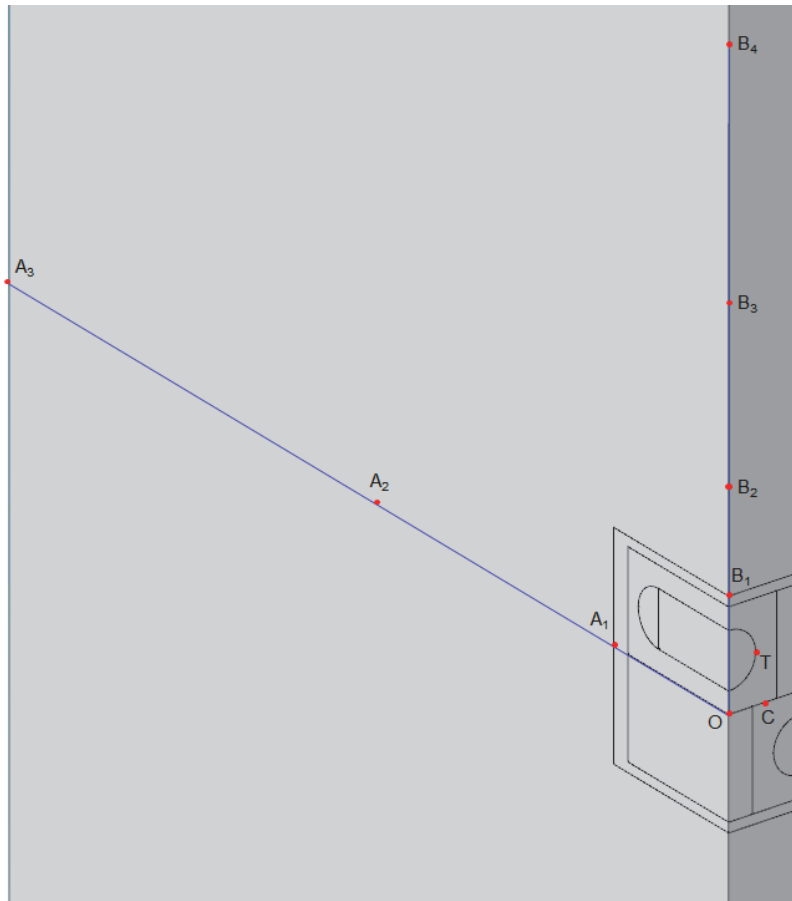


Figure 6: Locations at Which the Near-field Modelling Results will be Output in this Report

4.1.2 Near-Field Model Boundary Conditions

Thermal Boundary Conditions shown in Figure 4 are:

- The temperature on the top surface (ground surface) is 5°C (Baumgartner et. al. 1994).
- An isothermal condition is applied at bottom of the model (i.e., 10,000 metres below ground surface) at a temperature of 125°C (Baumgartner et. al. 1994).
- An adiabatic condition is applied on the four vertical surfaces of the model due to mirror symmetry. This represents the thermal conditions associated with this unit cell within an infinite tabular array of placement rooms.
- A uniform thermal load is applied at the volume of two one-fourths of a container. The total thermal load applied is one half (1/2) of a container thermal load (Table 1) due to the intersection of two adiabatic planes at the container centreline.

The thermal boundary conditions described above represent boundary conditions for a unit cell in a horizontally infinite repository. Based on the study in Guo (2007), the results from the Near-Field Model using such boundary conditions are accurate for early times, and overestimated at long times.

4.1.3 Near-Field Model Initial Conditions

The initial ambient temperature of the model is based on a geothermal gradient of $0.012^{\circ}\text{C}/\text{m}$ of depth and a ground surface temperature of 5°C resulting in an ambient temperature of 125°C at the bottom of the model (i.e., at a depth of 10,000 m) (Baumgartner et. al. 1994).

4.2 MODELLING RESULTS FROM THE NEAR-FIELD MODEL

Figure 7 shows the temperatures in the rock along the vertical surface near the placement room after 45 years. The temperature around the tunnel is very uniform.

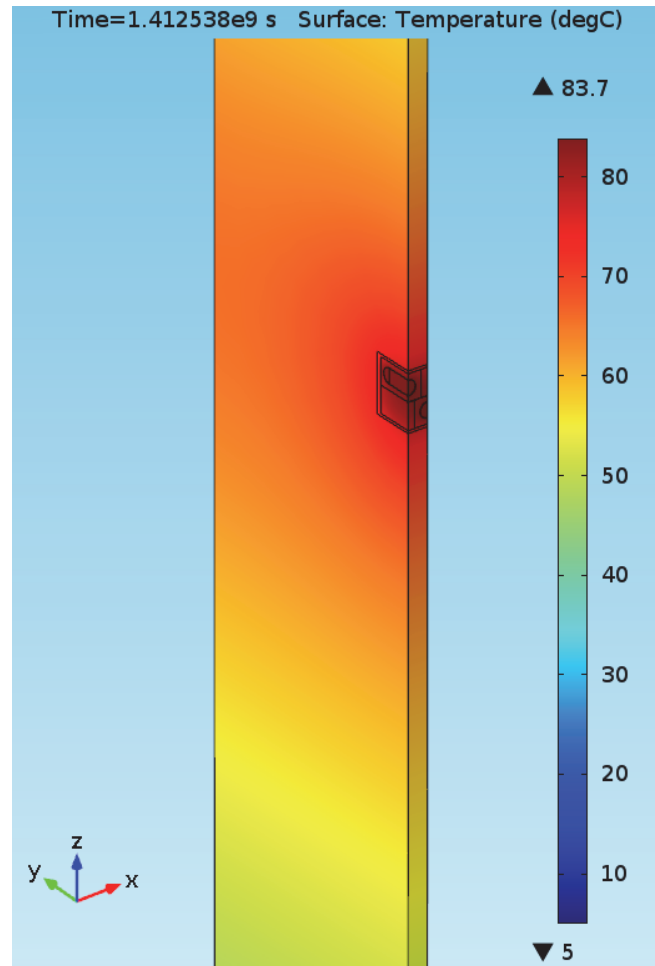


Figure 7: Temperatures in the Rock along the Vertical Surfaces near the Tunnel at Time of 45 Years after Placement

Figure 8 shows the temperatures along the horizontal cross-sections through the axis of the used fuel container after 45 years. The maximum container temperature of 84°C is reached at this time.

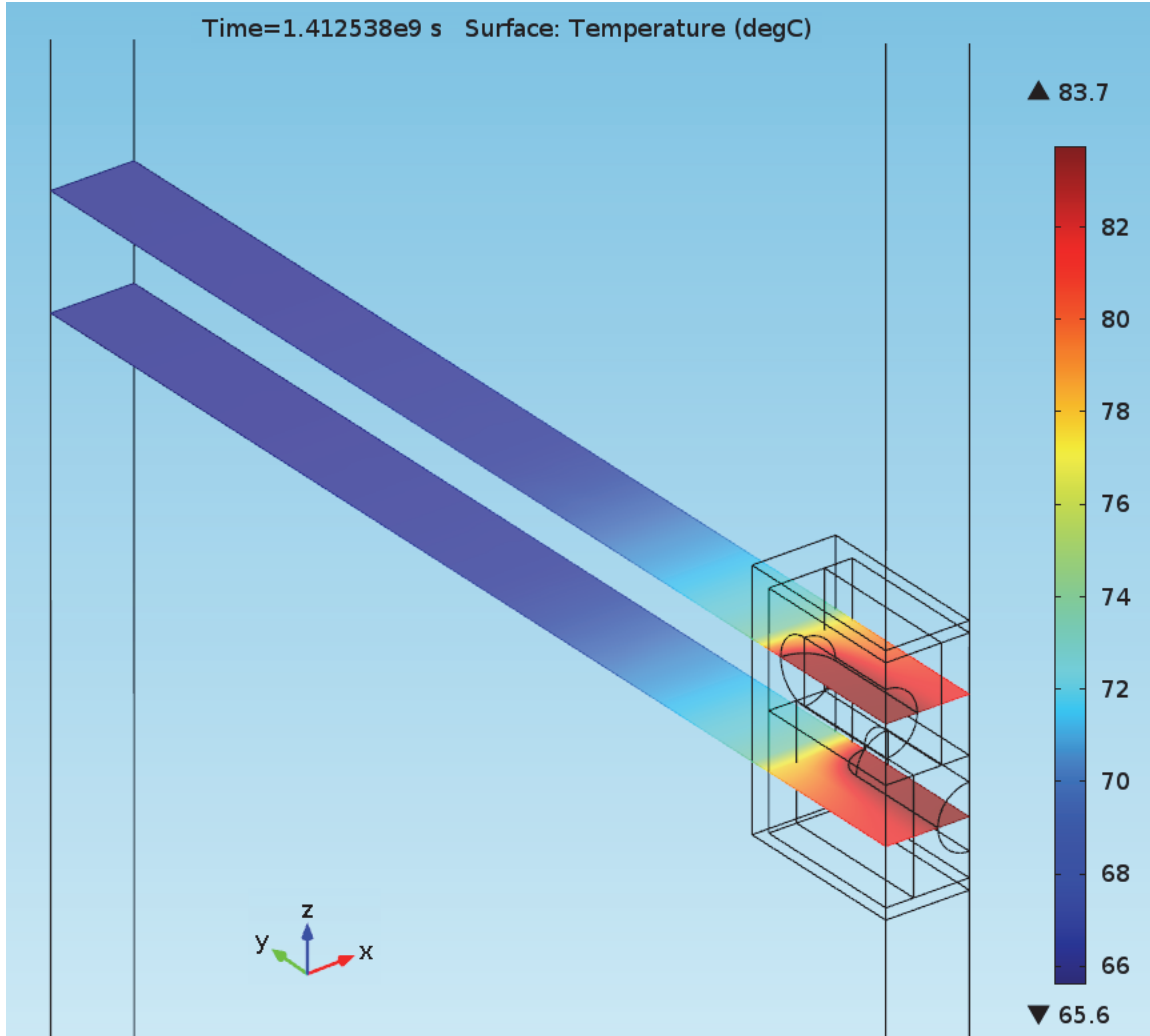


Figure 8: Temperatures in the Rock along the Horizontal Cross-sections through the Container Axis at Time of 45 Years after Placement

Figure 9 shows the temperature as a function of time at five points along vertical line OB₄. The temperature at Point O, which is the tunnel centre below the upper layer container, reaches a peak of 83°C at 45.8 years after placement and then reaches a second peak of 83°C at 1,480 years. The temperature at the roof of the placement tunnel (Point B₁) reaches 77°C at 65 years and 82°C at 1,550 years. After 1,590 years, the temperature at 1.0 m above the tunnel roof (B₂) reaches 74°C at 76 years and then 81°C. After 1,660 years, the temperature at 5 m (B₃) and 10 m (B₄) from the tunnel centre O reaches 80°C and 79°C.

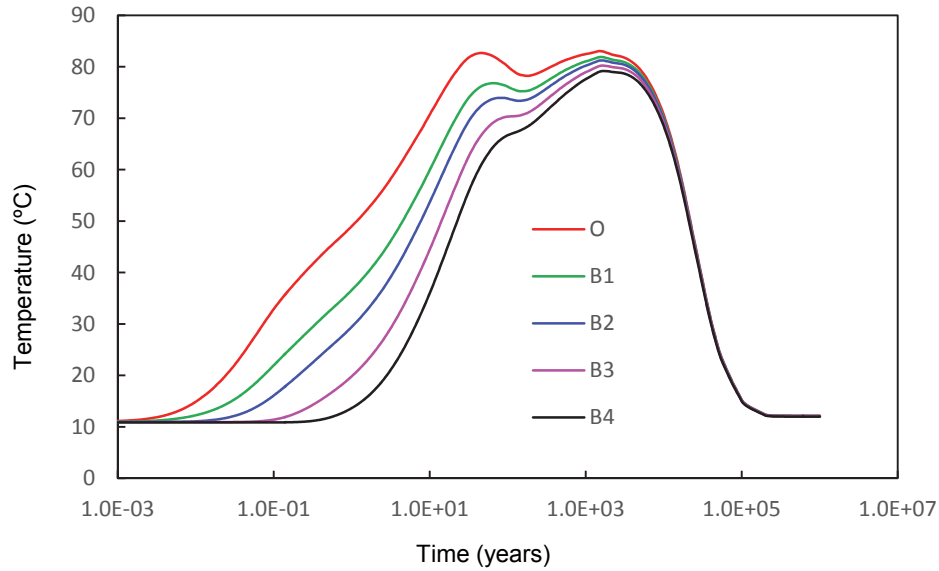


Figure 9: Temperature at Points O, B₁, B₂, B₃ and B₄

Figure 10 shows the temperature as a function of time at points O, A₁, A₂ and A₃. The temperature reaches 75°C at the wall of the placement tunnel (Point A₁) after 72.6 years, 71°C horizontally 5.0 m from the tunnel centre (A₂) after 90 years, and 70°C horizontally 10.0 m from the tunnel centre (A₃) after 90 years. After 1,550 years, the temperature reaches 82°C at the wall of the placement tunnel (Point A₁), 81°C horizontally 5.0 m from the tunnel centre (Point A₂), and 80°C horizontally 10.0 m from the tunnel centre (Point A₃).

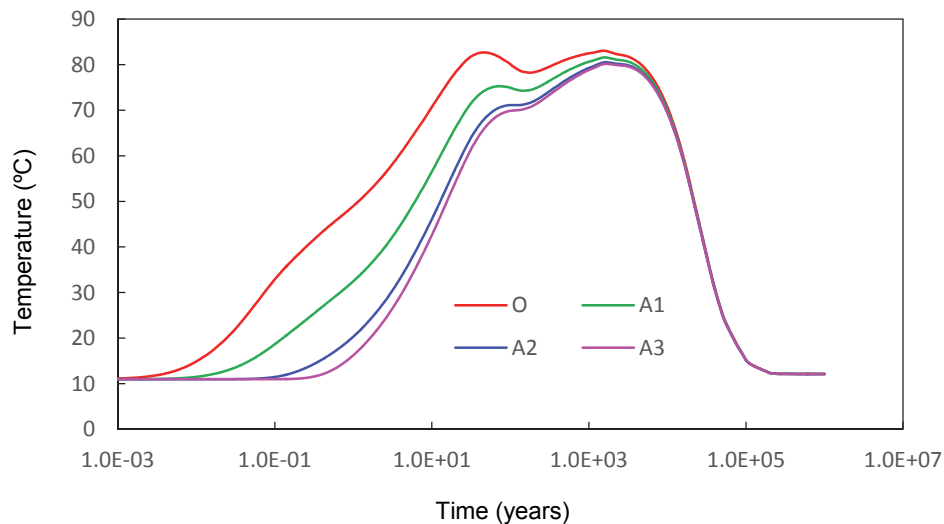


Figure 10: Temperature at Points O, A₁, A₂, and A₃

Figure 11 shows the temperature as a function of time at Points O, B₁, C and T. After 45 years of placement, the temperature reaches 84°C on the container surface (Point T) and 83°C at Point C. After 1,550 years, the temperature reaches 83°C on the container surface and 83°C at Point C.

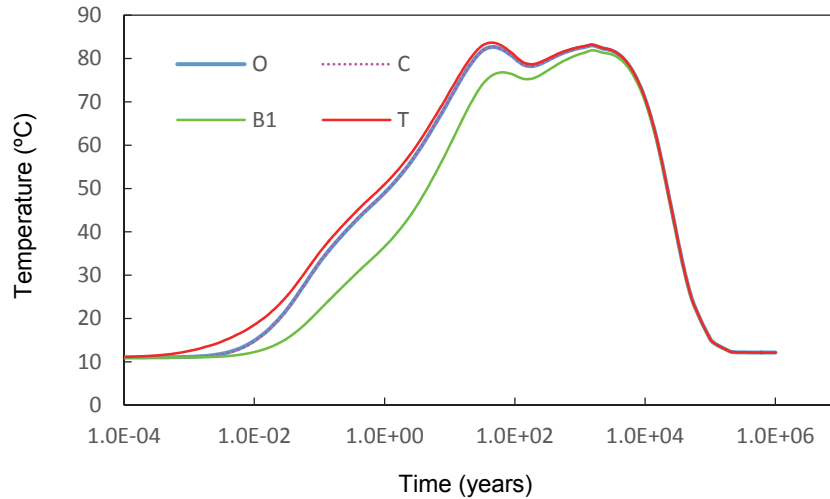


Figure 11: Temperature at Points O, C, B₁, and T

Figure 12 shows the temperature along horizontal line OA₃ at four different times. At different times, the thermal gradient in gap fill is the greatest because it has smallest value of thermal conductivity. With time, the temperature becomes more uniform.

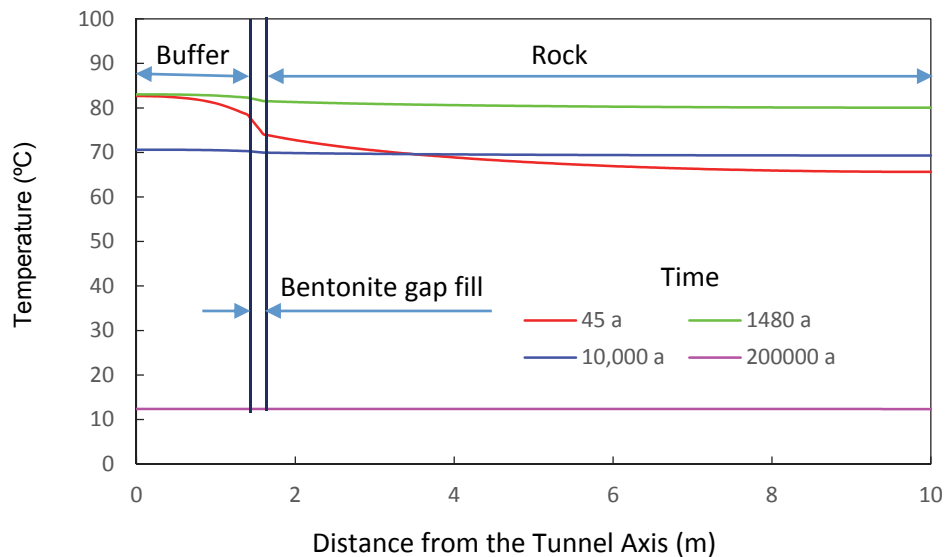


Figure 12: Temperature along the Horizontal Line OA₃ at Different times

In summary, the container surface temperature reaches its first peak of 84°C after 45 years and then reaches a second similar peak of 83°C after 1,550 years. The temperature at the tunnel centre reaches its first peak of 83°C after 45 years and then reaches a second peak of 83°C after 1,550 years. The rock temperature at the roof of the tunnel above the container reaches its first peak of 77°C after 65 years and its second peak of 82°C after 1,550 years. The rock temperature at the middle wall of the tunnel reaches its first peak of 75°C after 73 years and its second peak 82°C after 1,550 years.

These second peaks are influenced by the adiabatic boundary condition on the vertical surfaces and may therefore not be real. This is investigated further in later sections of this report.

5. THE FAR-FIELD MODEL

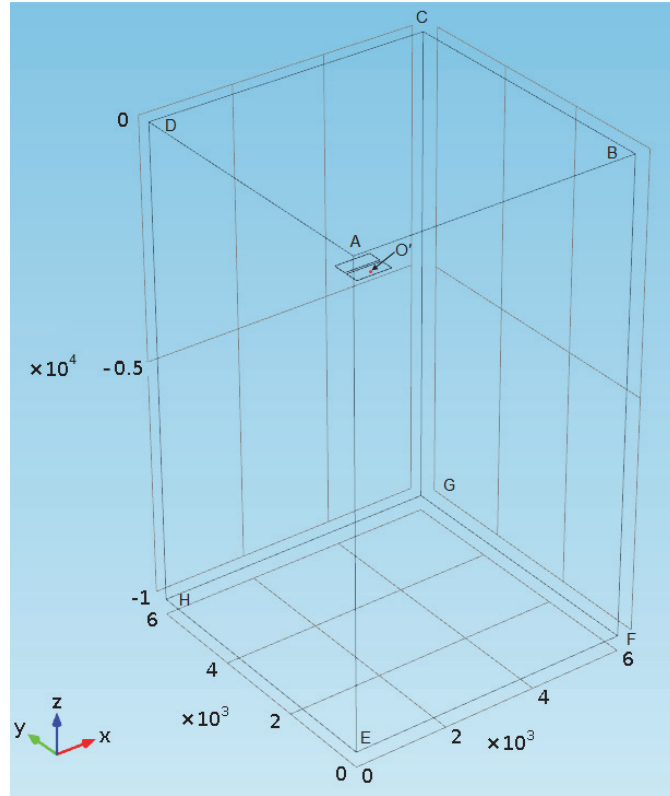
This section describes the Far-Field Model for a repository with a placement room spacing of 20 m (Figure 2) and a container spacing of 1.5 m in the same layer (Figure 3). This repository has 284 placement rooms in eight panels, with four panels each having 35 placement rooms and four panels each having 36 placement rooms (Figure 2). There are 375 buffer box positions available in each room. Conservatively, two 36 placement room panels with 375 containers in each room are chosen as the case for building the Far-Field Model. Therefore, the plan area of each panel is 720 m by 281.5 m. The depth of the placement room bottom from the ground surface is 500 m.

5.1 MODEL GEOMETRY, THERMAL BOUNDARY AND INITIAL CONDITIONS

The far-field thermal analysis provides an assessment of the thermal conditions in the rock mass surrounding a repository of finite dimension.

5.1.1 Far-Field Model Geometry

An isometric view of the far-field model is shown in Figure 13. Due to symmetry, only a one-quarter section of the repository is modelled. The model is bounded vertically by the ground surface on the upper side and by a plane 10,000 m below the ground surface at the bottom. The horizontal dimensions of the model in the X- and Y-directions are 6,000 m x 6,000 m. These dimensions should be sufficient such that the thermal response of the rock at the boundaries remains unaffected by the presence of the DGR during the simulation time period. One-quarter of the DGR is represented by two panels with a 2 m thick plate of material generating heat. The horizontal dimensions of one DGR panel are 720 m x 281.5 m as shown in Figure 14. The locations of each panel in the far-field model are also shown in Figure 14.



(Axis dimensions are in metres)

Figure 13: Isometric View of Far-Field Model

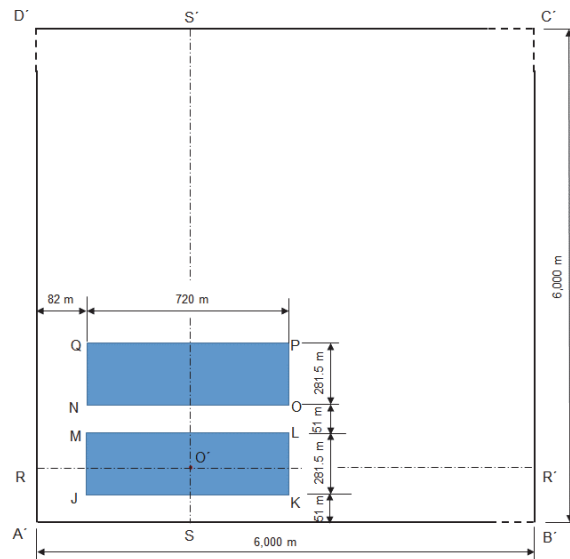


Figure 14: Cross Section of the Far-Field Model at Depth of 500 m from the Ground Surface

5.1.2 Far-Field Model Boundary Conditions

As with the Near-Field Model, the thermal boundary conditions are defined as follows.

- The upper surface boundary condition is modelled as an isothermal boundary, at a temperature of 5°C, representing the average Canadian Shield surface temperature.
- The lower boundary (i.e., 10,000 m below ground surface) is also modelled as an isothermal boundary set at a temperature of 125°C (Baumgartner et.al. 1994).
- The vertical boundaries are modelled as adiabatic planes of symmetry.
- The heat generated from the used-fuel containers in one-quarter of a repository is uniformly distributed throughout two panel plates (i.e., a rectangular plate of 720 m long by 281.5 m wide by 2.0 m high (2.0 m is the height of the two layers of buffer boxes)).

The model is representative of a finite size DGR positioned in an infinite extent of granite.

5.1.3 Far-Field Model Initial Conditions

The initial temperature of the model corresponds to a geothermal gradient of 0.012°C/m of depth, with the ground surface temperature at 5°C and the model bottom temperature at 125°C (Baumgartner et. al. 1994).

5.1.4 Finite Element Discretization

The finite-element discretization of the far-field model is shown in Figure 15. The domain is discretized such that the elements are more densely distributed in the rock mass just above and beneath the repository level where the thermal gradients are expected to be the greatest. The model has 99,465 tetrahedral elements.

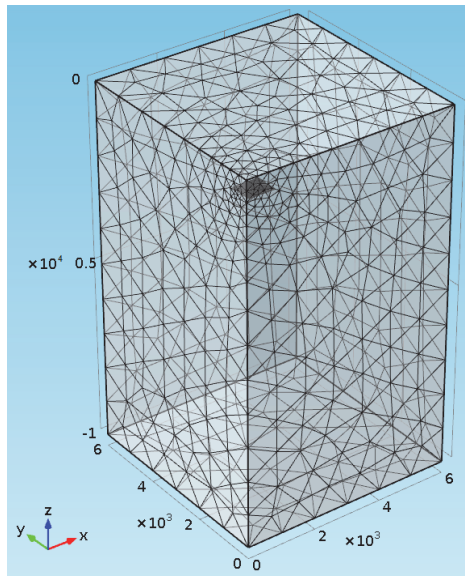


Figure 15: Mesh for the Far-Field Thermal Model

5.2 NUMERICAL RESULTS FROM FAR-FIELD MODELLING

Figure 16 and Figure 17 show the isometric view of the temperature after 78 years and 700 years of used-fuel container placement. Figure 18 and Figure 19 show the temperature along the vertical cross section through line S-S' after 78 years and 700 years. Figure 20 and Figure 21 show the temperature along the vertical cross section through line R-R' after 78 years and 700 years. Figure 22 and Figure 23 show the temperature along the horizontal cross section at a depth of 500 m from the ground surface after 78 years and 700 years. The peak temperature at repository level is 71°C after 78 years and 67°C after 700 years, occurring at Point O' (for location to see Figure 14).

These results differ from similar results obtained with the Near-Field Model described in Section 4 because the Near-Field Model is built with more detail for used-fuel containers, engineered sealing materials and rock. The Near-Field Model also determines the thermal response of the unit cell located within a panel at Point O' (see Figure 14 for location) assuming an infinite repository.

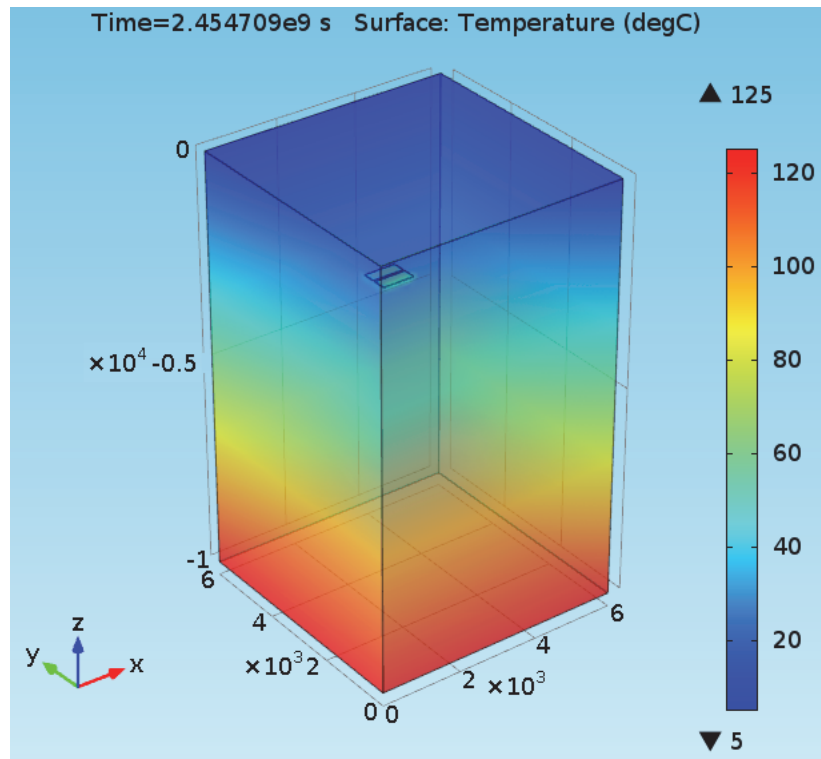


Figure 16: Isometric View of Temperature in the Far-Field Model at 78 Years after Placement

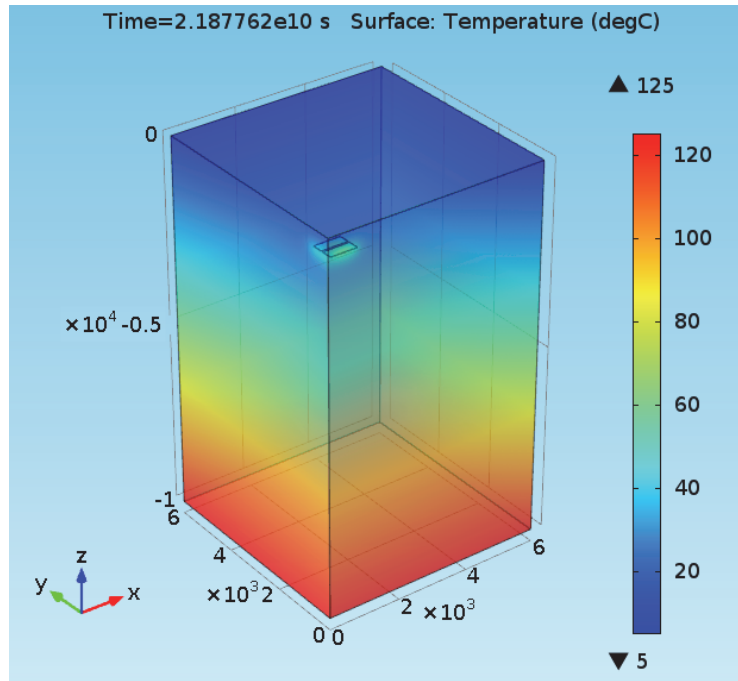


Figure 17: Isometric View of Temperature in the Far-Field Model at 700 Years after Placement

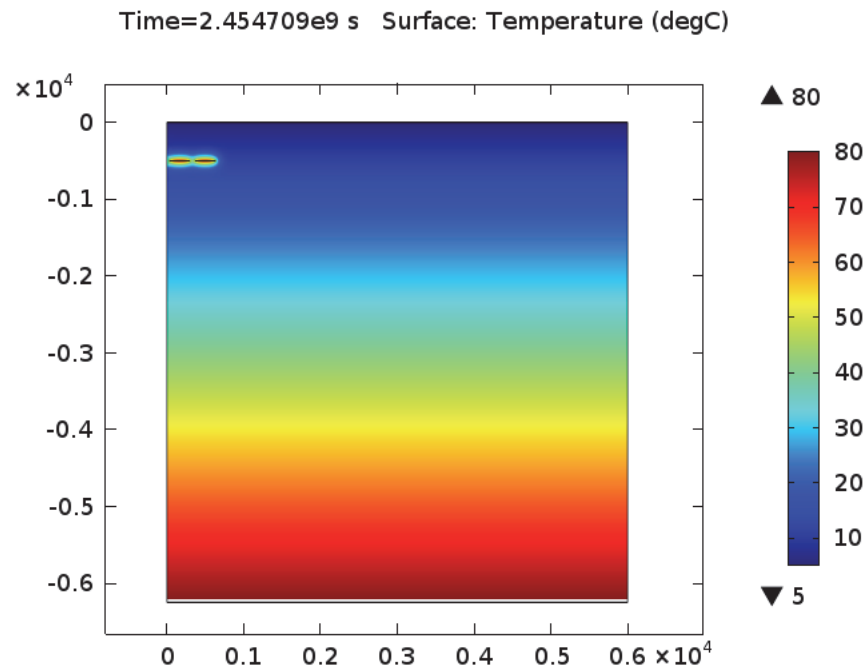


Figure 18: Temperature along Vertical Cross Section through Line S-S' at 78 Years after Placement

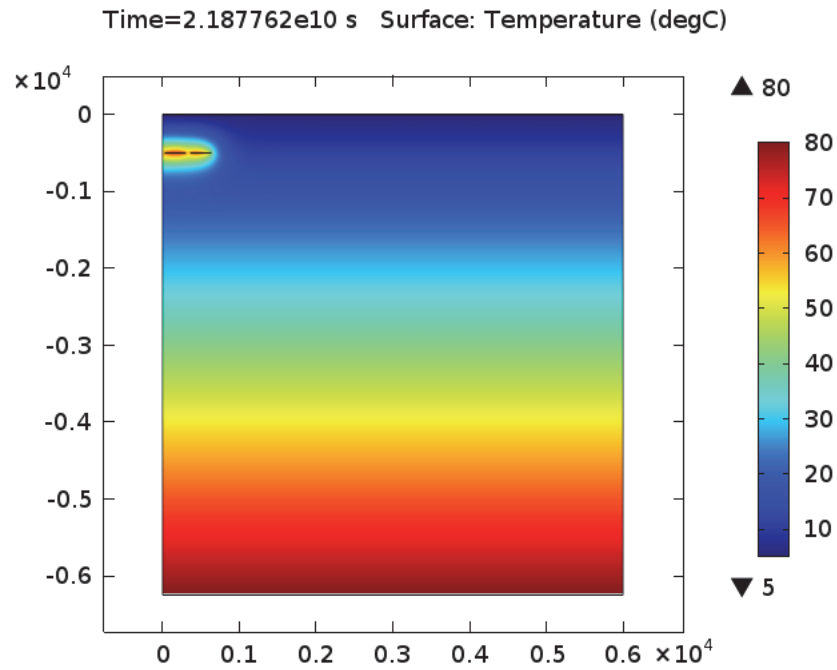


Figure 19: Temperature along Vertical Cross Section through Line S-S' at 700 Years after Placement

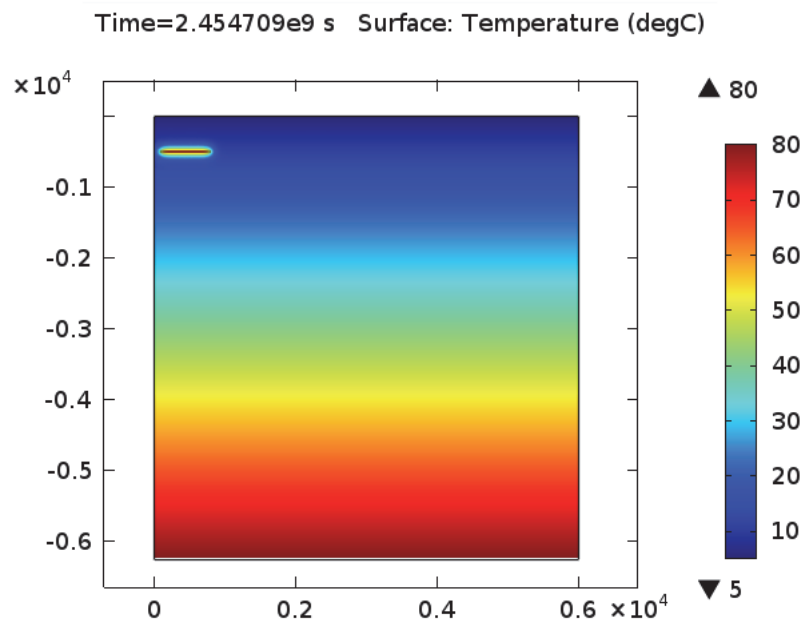


Figure 20: Temperature along Vertical Cross Section through Line R-R' at 78 Years after Placement

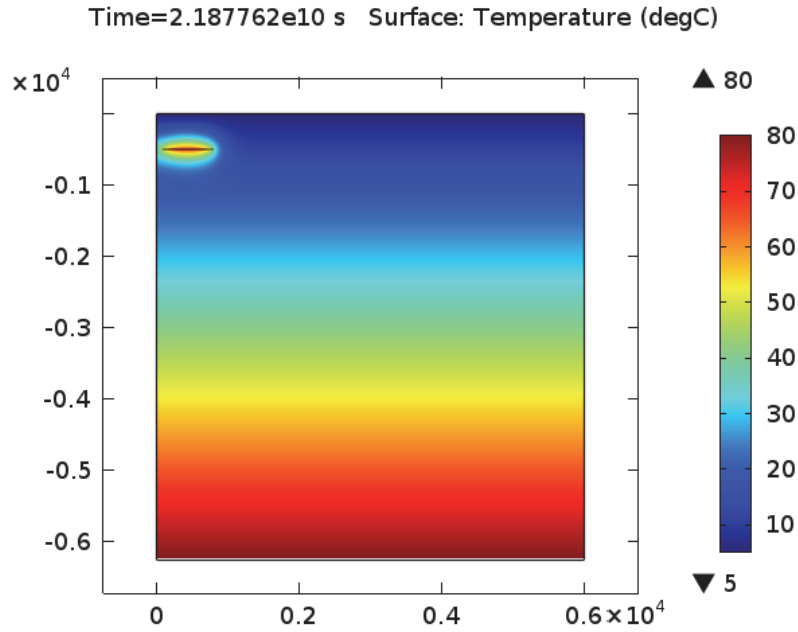


Figure 21: Temperature along Vertical Cross Section through Line R-R' at 700 Years after Placement

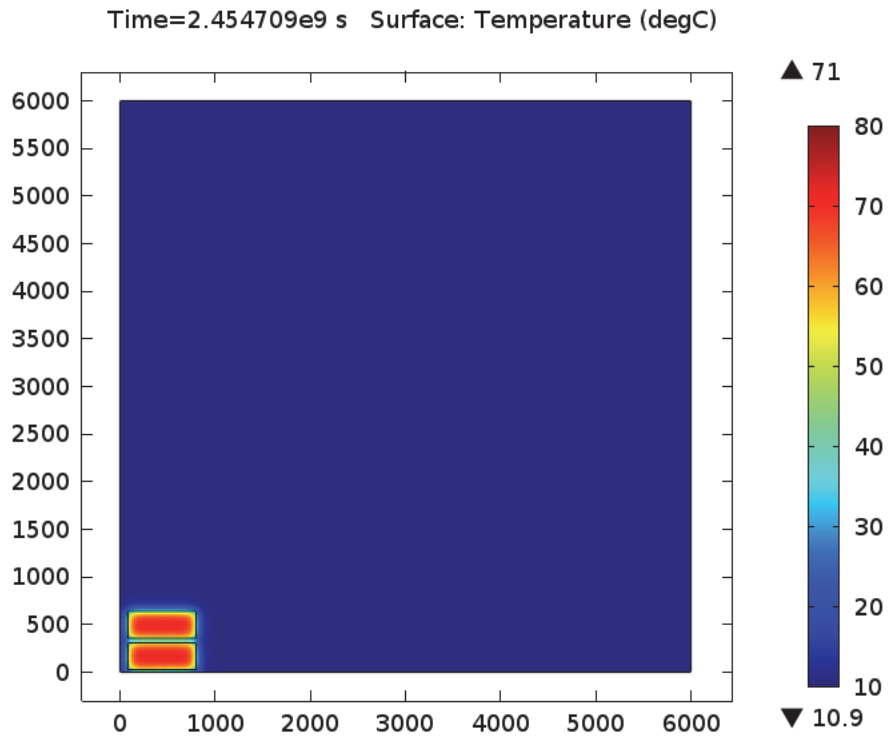


Figure 22: Temperature along Horizontal Cross Section at a Depth of 499 m at 78 Years after Placement

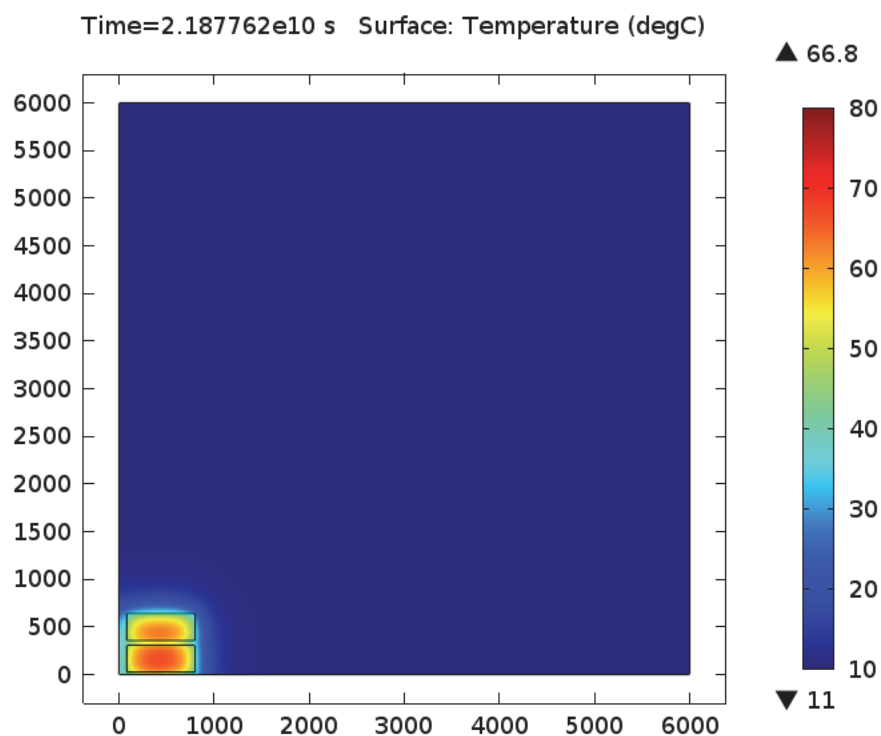


Figure 23: Temperature along Horizontal Cross Section at a Depth of 499 m at 700 Years after Placement

Figure 24 illustrates the temperatures at locations O', P, L, A' and B' (for locations see Figure 14). The peak temperature occurs at 78 years at the panel centre (Point O') with a magnitude of 71°C. The maximum Far-Field Model temperature is lower than the highest Near-Field Model temperature (84°C) shown in Figure 11 because the modelled far-field temperature represents the average temperature in a volume of 10 m x 0.75 m x 2.0 m of rock located in the Near-Field Model at a depth of 500 m. The peak temperatures at the panel' corners are 36°C (Point L) after 830 years and 27°C (Point P) after 600 years. The peak temperatures predicted at the centre of the repository (Point A') and the corner of the far-field model (Point B') are 43°C after 2,200 years and 11°C, respectively. The absence of temperature change at the model boundary (Point B') during one million years indicates that the horizontal dimensions are sufficiently large.

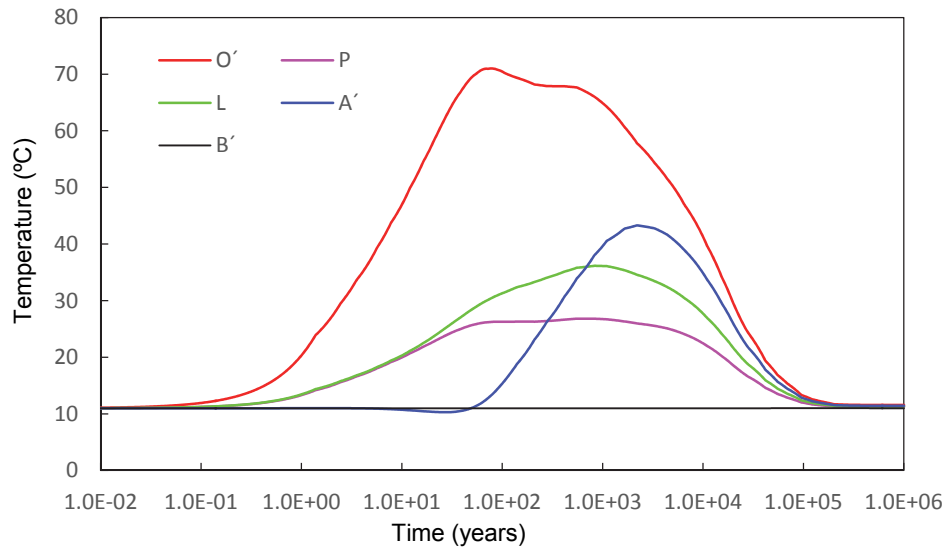


Figure 24: Temperature as a Function of Time at Different Points at Repository Level from Far-Field Model

Figure 25 shows the temperature as a function of time at different depths along the axis of the repository. The temperature at a depth of 5,000 m is unchanged, indicating that the vertical dimension of 10,000 m is sufficient.

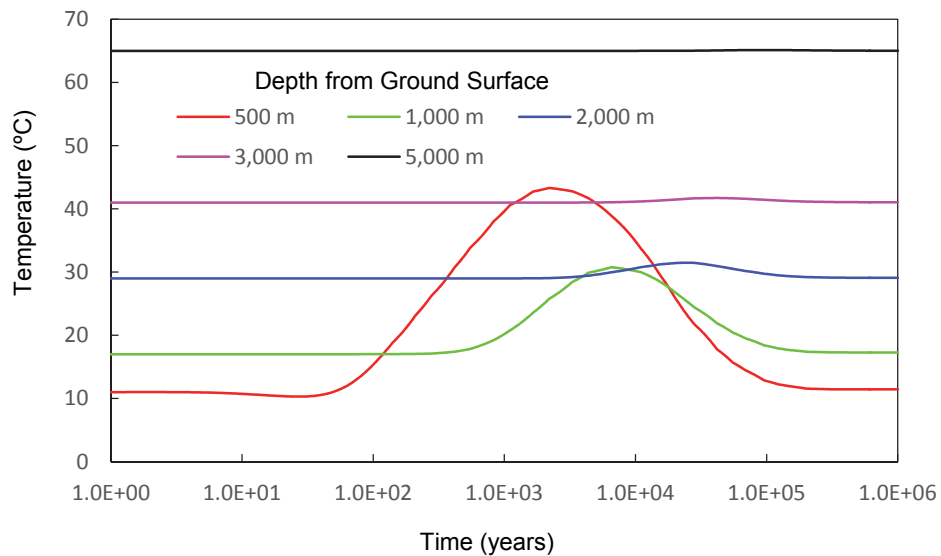


Figure 25: Temperature as a Function of Time at Different Points along the Vertical Line through the Repository Centre

Temperature profiles along the horizontal lines RR' and SS' (refer to Figure 14 for location) at four different times are shown in Figure 26 and Figure 27. The thermal load caused by used nuclear fuel influences the temperature of the rock in a range of 2,000 m or less from the centre of the repository. Therefore, the horizontal dimension of 6,000 m in the model is sufficient for the far-field model.

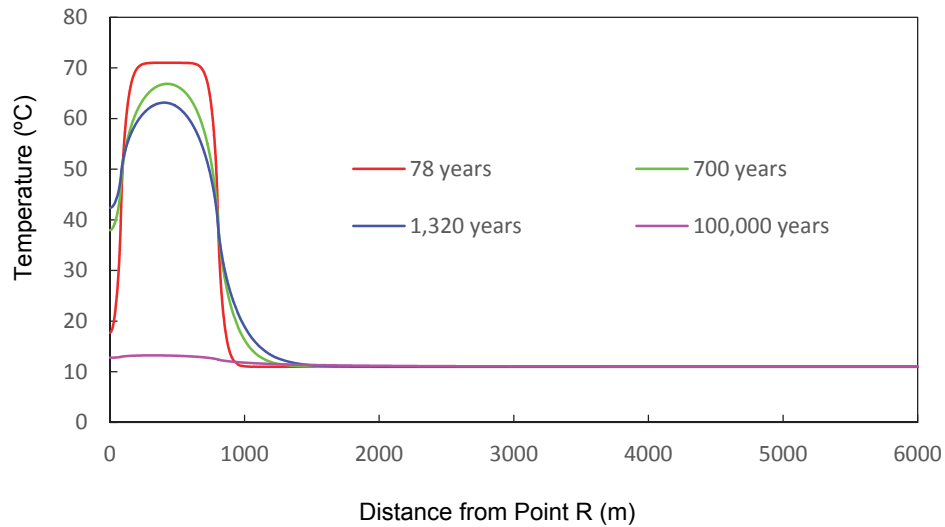


Figure 26: Far-Field Temperature Profiles at Different Times along Horizontal Line RR'

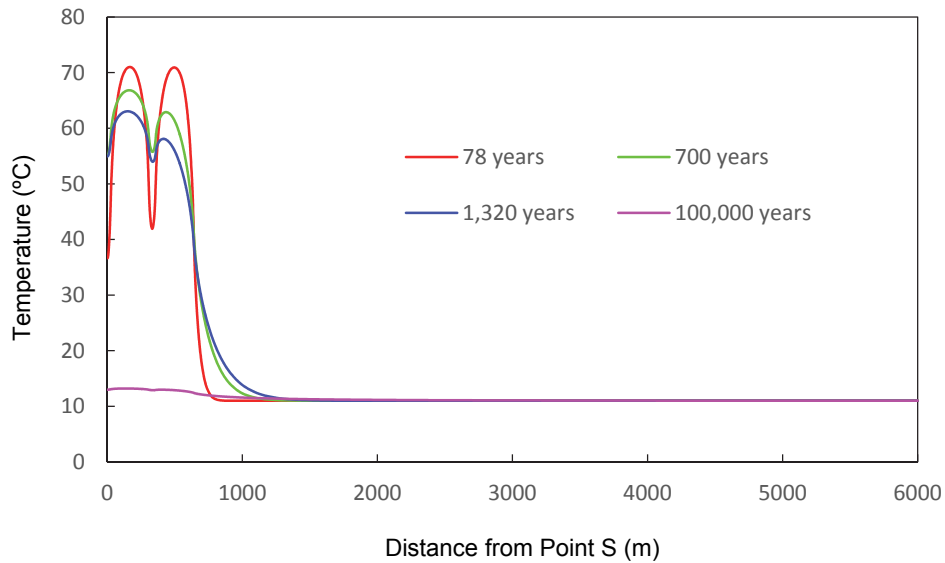


Figure 27: Far-Field Temperature Profiles at Different Times along Horizontal Line SS'

Figure 28 shows the far-field temperature profiles along vertical symmetry line AE. The thermal load caused by the used nuclear fuel influences the temperature of the rock in a range of 3,000 m or less below the centre of the repository.

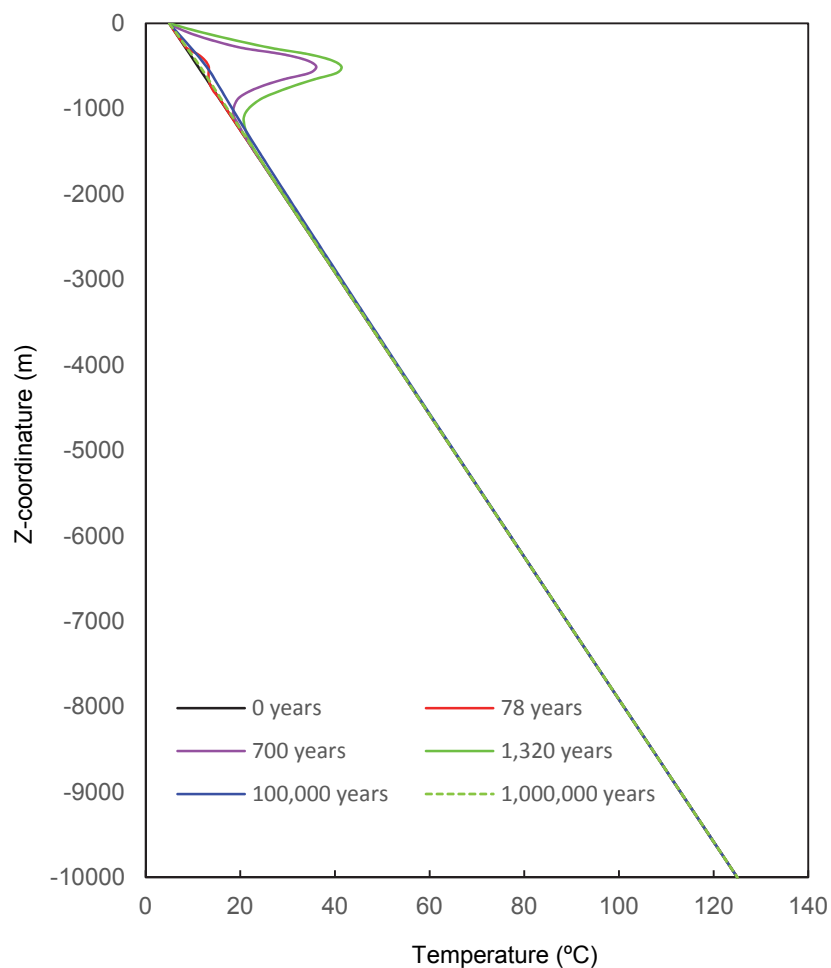


Figure 28: Far-Field Temperature Profiles at Different Times along Vertical Symmetry Line through the Repository Centre

In summary, the maximum temperature in the repository is 71°C occurring at the centre of Panel B (Point O') after 78 years of used-fuel container placement. The peak temperature of the repository centre is 43°C. The heat load in the crystalline repository thermally only influences the rock horizontally 2~3 km and vertically 5 km from the repository centre.

6. INFLUENCE OF THE ADIABATIC BOUNDARY CONDITION IN THE NEAR-FIELD MODEL

To examine the influence of thermal boundary conditions on the Near-Field Model, a Simplified Near-Field Model was built in which the boundary conditions and initial conditions are the same as the boundary conditions applied in the Near-Field Model. In the Simplified Near-Field Model, the heat load is applied in the volume of the block with dimensions of 0.75 m x 10.0 m x 2.0 m located at a depth of 500 m. The Simplified Near-Field Model contains only one kind of material (rock) as in the Far-Field Model. This approach ensures the method of applying the heat load is the same as that in the Far-Field Model. The Simplified Near-Field Model represents a repository with infinite horizontal dimensions, while the Far-Field Model in Section 5 represents a repository with finite horizontal dimensions.

This section describes the Simplified Near-Field Model and its thermal response together with the difference in thermal results between the Far-Field Model and the Simplified Near-Field Model. The temperature difference along the vertical line through the panel centre (O') between the two models represents the influence of the thermal boundary conditions applied to the four vertical surfaces in the Near-Field Model.

These analyses are done using the Far-Field Model and the Simplified Near-Field Model rather than the Near-Field Model because it is not practical to expand the near-field unit cell detail to the scale of the entire repository.

6.1 SIMPLIFIED NEAR-FIELD MODEL

6.1.1 Simplified Near-Field Model Geometry

Figure 29 illustrates the Simplified Near-Field Model geometry, in which the thermal load per volume of the repository is the same as used in the panels in the Far-Field Model (Figure 13). Due to symmetry, horizontal dimensions of 10 m x 0.75 m are selected as shown in Figure 29. The repository is represented by a 2 m-thick plate located at depth of 500 m from the ground surface.

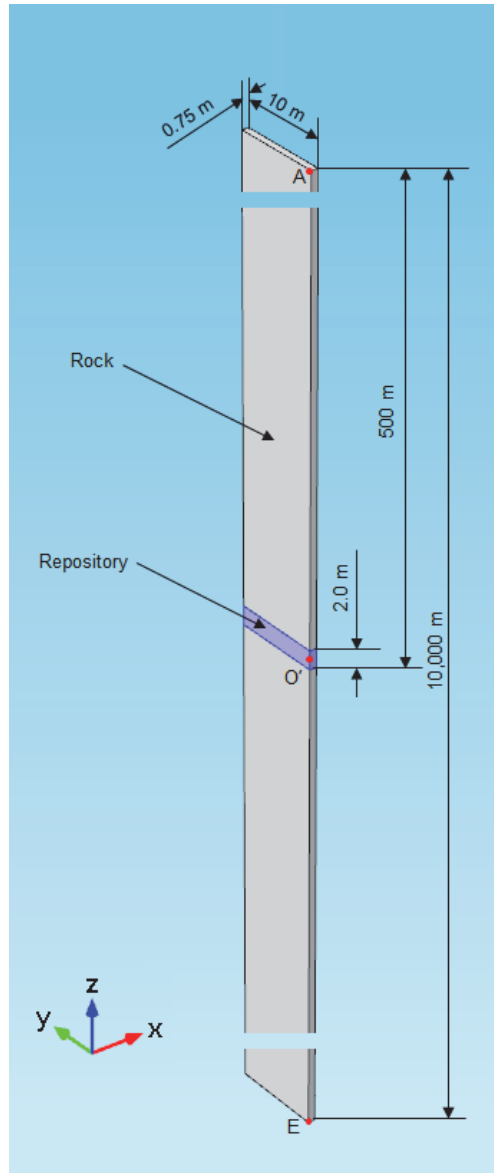


Figure 29: Simplified Near-Field Model Geometry

6.1.2 Boundary Conditions for the Simplified Near-Field Model

As with the Near-Field Model, the thermal boundary conditions are defined as follows.

- The upper surface boundary condition is modelled as an isothermal boundary, at a temperature of 5°C , representing the average Canadian Shield surface temperature.
- The lower boundary is also modelled as an isothermal boundary set at a temperature of 125°C , based on a geothermal gradient of 0.012°C/m of depth plus the ground surface temperature of 5°C .
- The vertical boundaries are modelled as adiabatic planes of symmetry.

- The same heat density applied on the panel plate in the Far-Field Model as shown in Figure 13 is applied on the repository plate in Figure 29 (i.e., the total heat source is the same as that applied at the Near-Field Model shown in Table 1).

The model is representative of a DGR positioned in an infinite extent of granite.

6.1.3 Initial Conditions for the Simplified Near-Field Model

The initial temperature of the model corresponds to a geothermal gradient of $0.012^{\circ}\text{C}/\text{m}$, with the ground surface temperature at 5°C and a model bottom temperature at 125°C (Baumgartner et. el. 1994).

6.1.4 Finite Element Discretization

The finite-element discretization of the Simplified Near-Field Model is shown in Figure 30. The domain is discretized such that elements are more densely distributed in the rock mass just above and beneath the repository level where the thermal gradients are expected to be the greatest. The model has 85,920 elements.

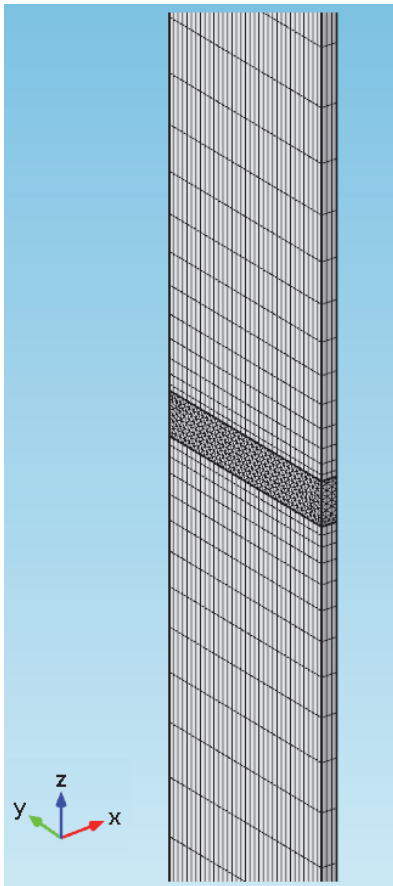


Figure 30: Mesh near the Repository in the Simplified Near-Field Model

6.2 NUMERICAL RESULTS FROM SIMPLIFIED NEAR-FIELD MODEL

Figure 31 and Figure 32 show the temperature in the rock from the Simplified Near-Field Model at 78 years and 1,320 years after placement of the used-fuel containers. The temperature at the repository level is 71°C at 78 years and 78°C at 1,320 years.

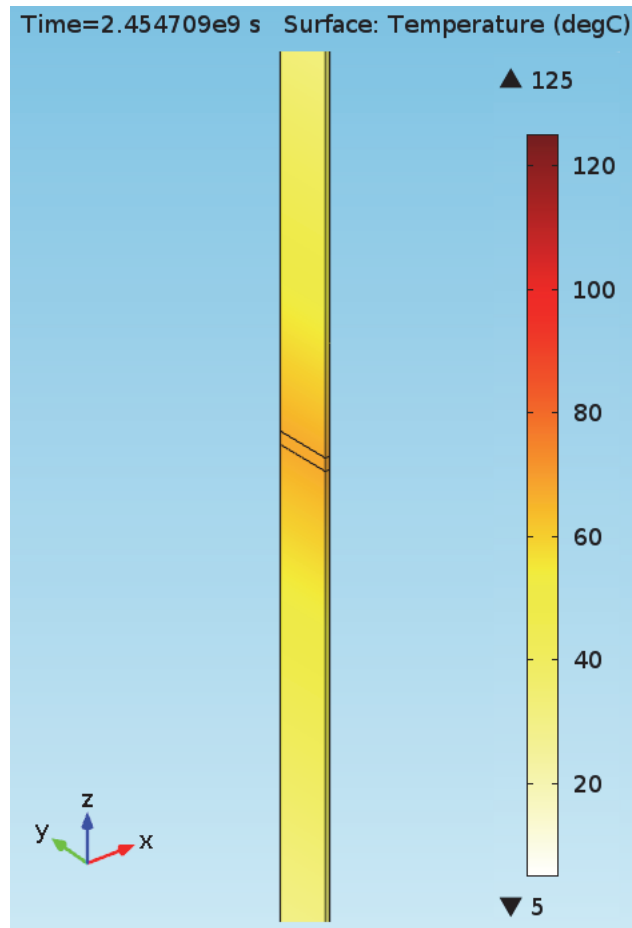


Figure 31: Isometric View of Temperature in the Simplified Near-Field Model at 78 Years after Placement

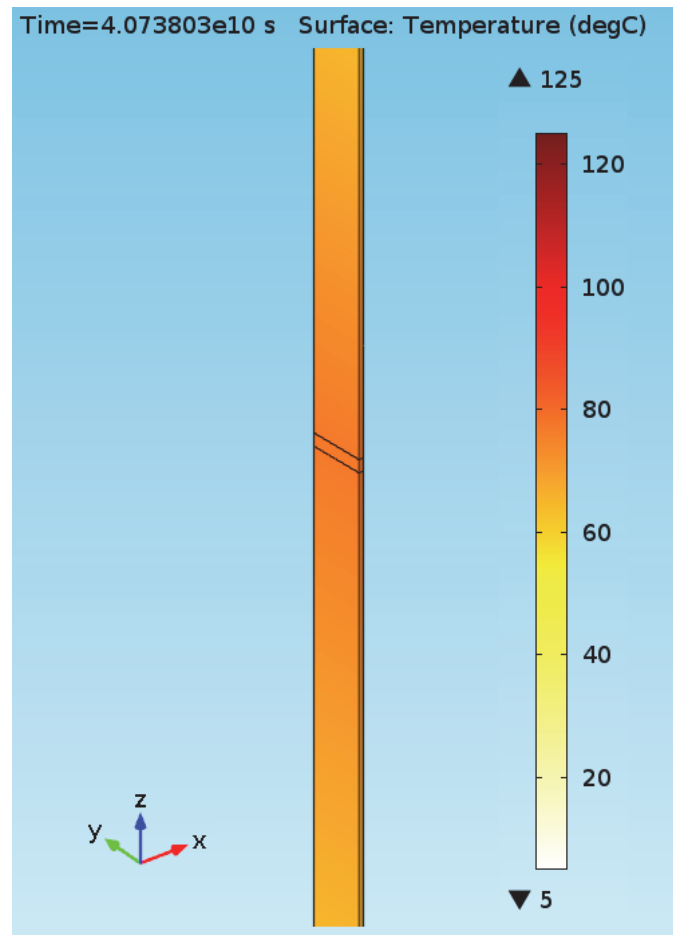


Figure 32: Isometric View of Temperature in the Simplified Near-Field Model at 1,320 Years after Placement

Figure 33 shows the temperature as a function of time at six different depths. At 500 m from the ground surface, the temperature reaches a peak of 72°C after 100 years, and reaches a second peak of 78°C after 1,320 years. At a depth of 9,000 m, the temperature increase is only 0.7°C after 295,000 years, indicating that the depth of 10,000 m is sufficient for the Simplified Near-Field Model.

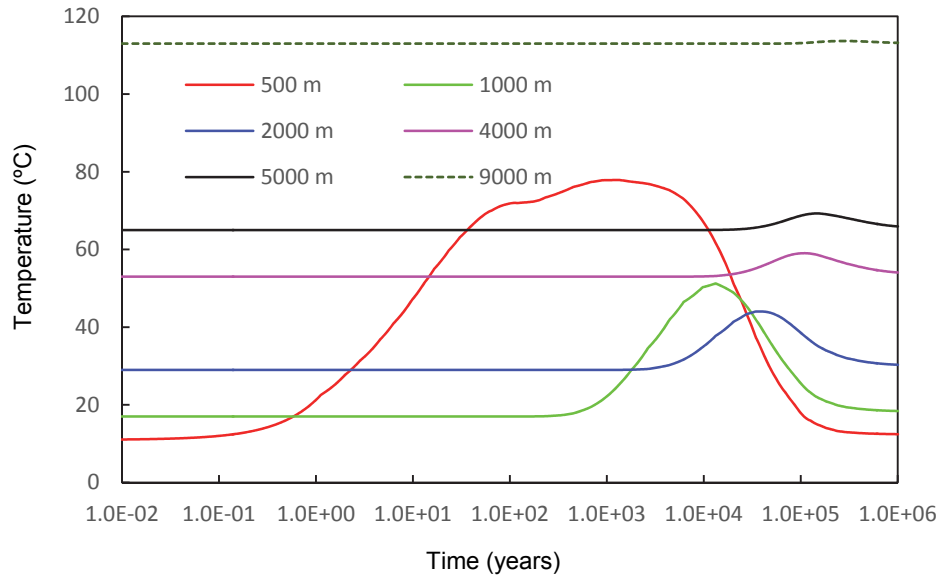


Figure 33: Temperature as a Function of Time at Different Depths

Figure 34 shows the temperature profiles along vertical line AE. This shows that the thermal response caused by the heat load from the horizontally infinite repository only reaches the depth less than 3,000 m during the first 10,000 years.

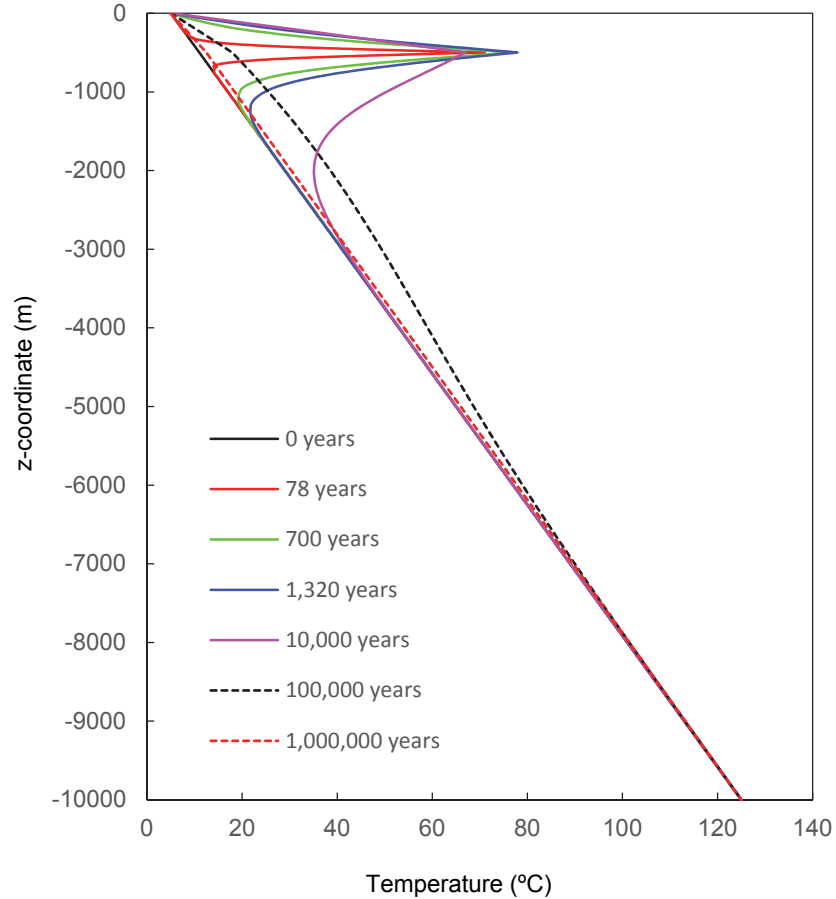


Figure 34: Temperature along Line AE at Different Times from the Simplified Near-Field Model

6.3 INFLUENCE OF THE BOUNDARY CONDITIONS IN THE NEAR-FIELD MODEL

Figure 35 shows the temperature difference at panel centre, O', between the Far-Field Model and the Simplified Near-Field Model. The Far-Field Model results represent the temperature changes induced by the heat load from the eight panels in the repository, while the temperatures for the Simplified Near-Field Model are caused by heat load not only from the eight panels but also from locations beyond the eight panel area (recall that the Simplified Near-Field Model is representative of an infinite repository). The difference in temperatures is therefore representative of the boundary condition effect on the Simplified Near-Field Model, and this difference can be subtracted from the Near-Field Model results to remove the effect of the boundary condition. The maximum temperature difference reaches 26°C after 10,000 years.

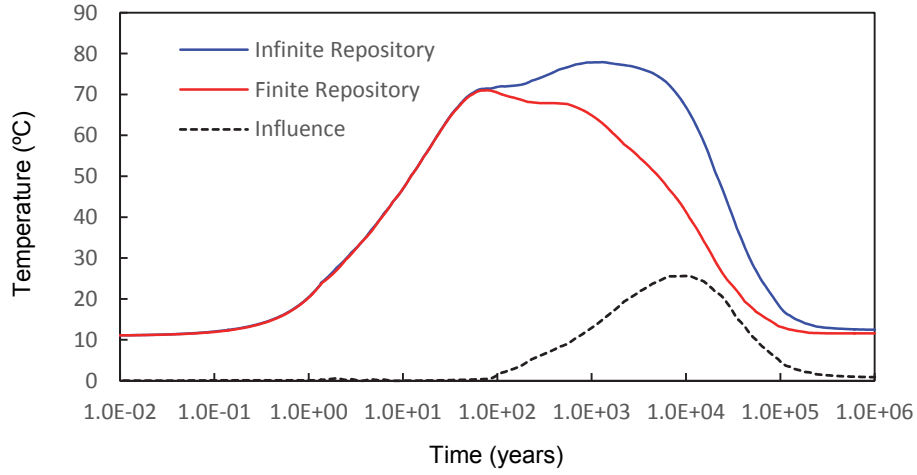


Figure 35: Temperature at Panel Centre from the Far-field Model with Horizontally Finite-Dimensional Repository and Temperature at Repository Depth from the Simplified Near-Field Model and their Differences

Figure 36 shows temperature difference profiles along a vertical line through panel centre O' between the Far-Field Model and the Simplified Near-Field Model. The temperature difference changes not only with time but also with depth. It can be expressed as:

$$\Delta T = \Delta T(t, z) \quad (1)$$

in which ΔT is the temperature difference at section centre between the Far-Field Model and the Simplified Near-Field Model, °C; t is time, second; z is the depth from the ground surface, m.

The Near-Field Model results can be modified by subtracting the temperature difference (Equation (2)) to erase the influence of the adiabatic boundary conditions:

$$T_m = T_n - \Delta T \quad (2)$$

in which T_m is the modified temperature based on near-field modelling results, °C; T_n is the results from the Near-Field Model.

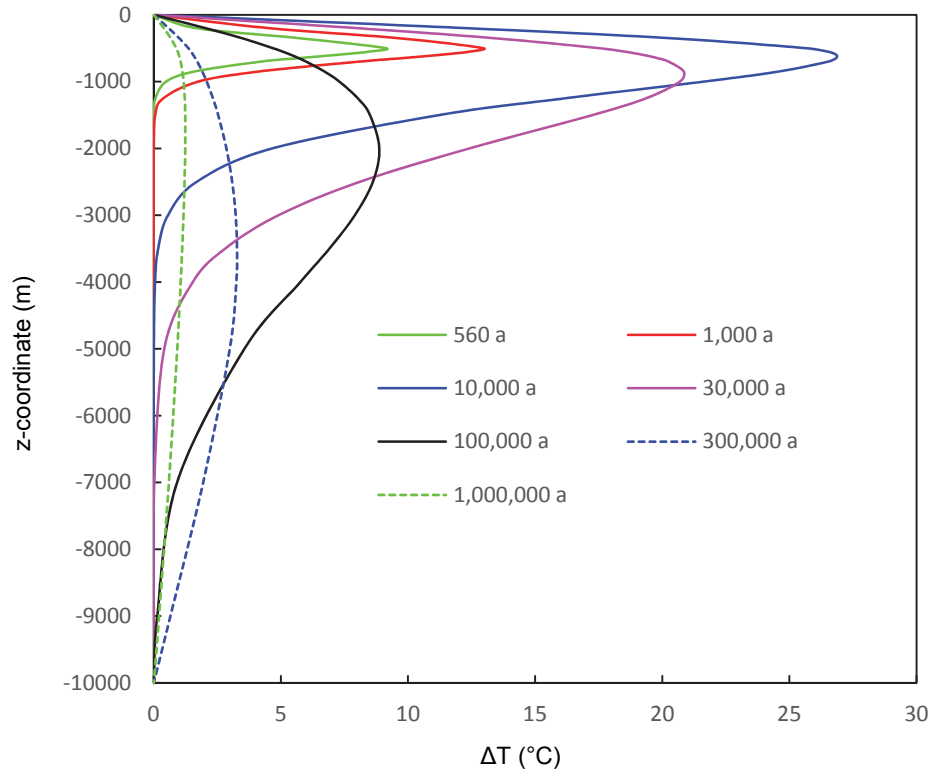


Figure 36: Temperature Difference Profiles along Vertical Line through Panel Centre O' between the Simplified Near-Field Model and the Far-field Model

Theoretically, the method can be applied to obtain the temperature for a unit cell at any location in the repository panels. However, the modified analysis is useful to apply to a unit cell at the panel centre as this is expected to be the hottest point in the repository

6.4 MODIFIED TEMPERATURES AT CONTAINER SURFACE AND DIFFERENT LOCATIONS NEAR THE CONTAINER

Figure 37 shows the temperature comparison at the container surface and at the centre of the tunnel between the Near-Field Model results and the modified results. Solid lines are from the Near-Field Model and dashed lines are the modified results. The modified temperature for the second peak is much lower than the first peak values at both locations. The temperatures now decrease to 67°C at the container surface (Point T) and at the tunnel centre (Point C) after 1,550 years.

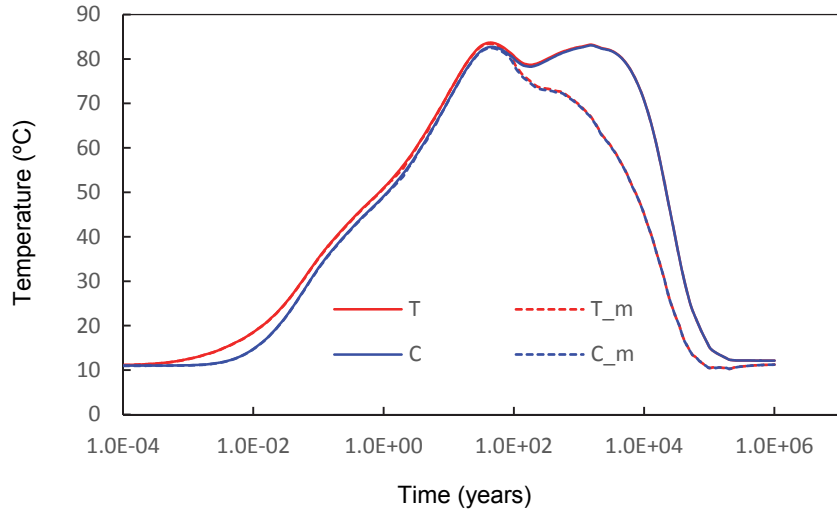


Figure 37: Comparison of the Temperature as a Function of Time at Points T (container surface) and Point C (centre of tunnel) between Near-Field Modelling Results and Modified Results

Figure 38 shows a comparison of temperature at Points O, B₁, B₂, B₃, and B₄, which are along the vertical line OB₄, between the near-field results and modified results. After 1,550 years, the temperatures from the modified results for Point O, B₁, B₂, B₃ and B₄ now decrease to 72°C, 70°C, 69°C, 68°C and 66°C.

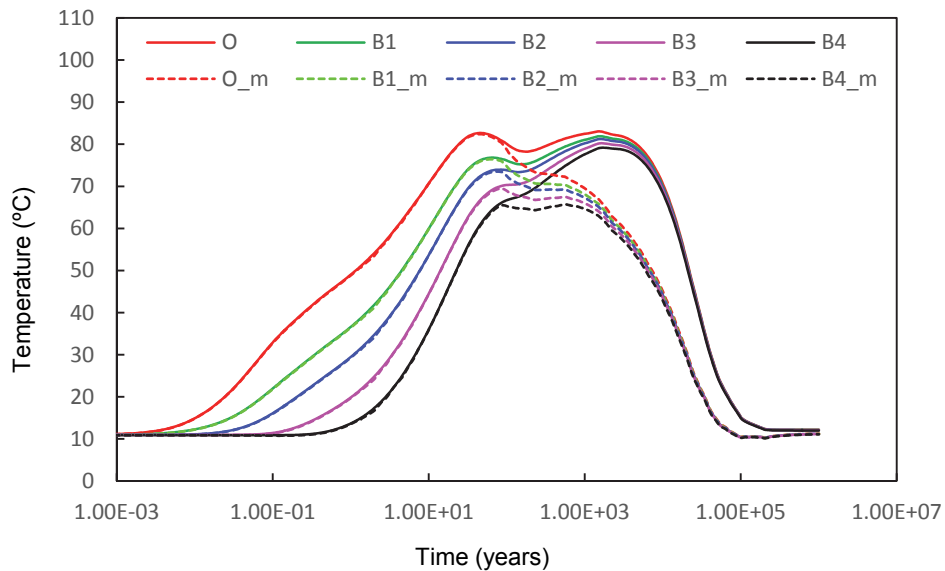


Figure 38: Comparison of the Temperature as a Function of Time at Points O, B₁, B₂, B₃ and B₄ between Near-Field Modelling Results and Modified Results

Figure 39 shows a comparison of temperature at Points O, A₁, A₂, and A₃, which are along the horizontal line OA₃, between the near-field results and modified results. After 1,550 years, the temperatures from the modified results for Point A₁, A₂, and A₃ are now 65°C, 64°C and 64°C.

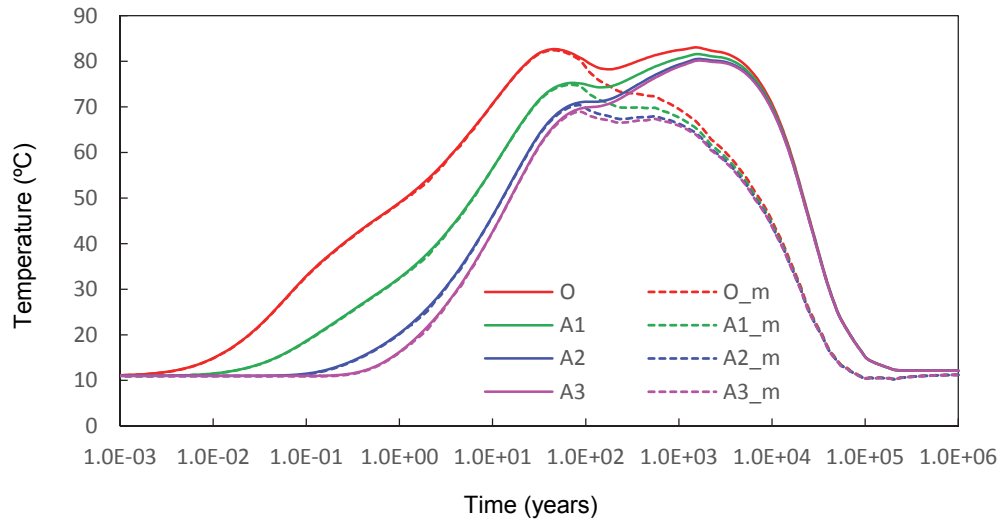


Figure 39: Comparison of the Temperature as a Function of Time at Points O, A₁, A₂ and A₃ between Near-Field Modelling Results and Modified Results

Figure 40 compares the temperature along Line AE after 10,000 years and 100,000 years from Near-Field Model to the modified results and its initial temperature. Below the depth of 4,000 m from the ground surface, there is no influence of heat source or the adiabatic boundary condition used in the Near-Field Model after 10,000 years. After 100,000 years, although the influence of the adiabatic boundary condition can reach a depth of 8,000 m from the ground surface, the influence of the heat source only reach a depth of 4,000 m from the ground surface.

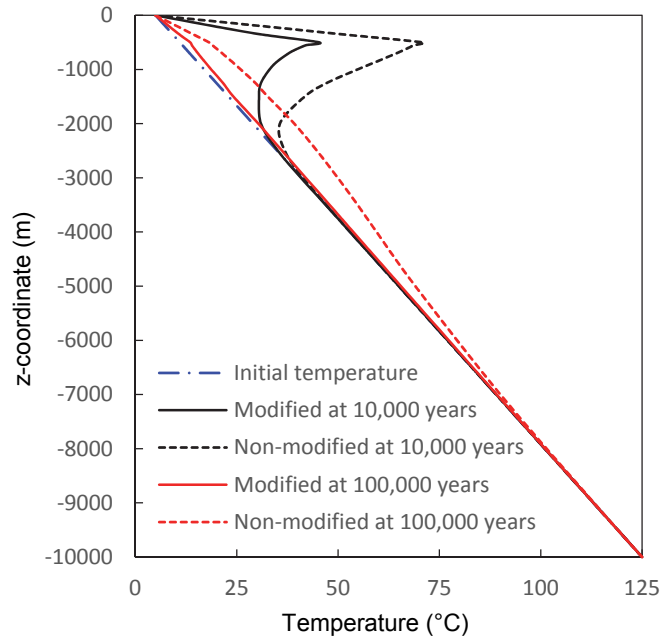


Figure 40: Comparison of Modified and Non-modified Temperature along Line AE after 10,000 Years and 100,000 Years from Near-Field Model with Initial Temperature

7. VALIDATION OF THE CORRECTION METHOD

To validate the method for correcting the influence of the adiabatic boundary condition applied in the Near-Field Model, COMSOL and the modification method is used to calculate the container temperature for the crystalline rock repository described in Baumgartner et al. (1994). This repository has horizontal dimensions of 1,740 m x 1,740 m located at a depth of 1,000 m of granite. It has 58 placement rooms with placement room spacing of 30 m. There are 3 containers across the width of a room and 798 containers across the length of a room. The container has a diameter of 0.63 m and a length of 2.117 m. Each container contains 1362.7 kgU with a burnup of 684 GJ/kgU.

The thermal response of this repository was calculated using the HOTROK analytical computer code (Baumgartner et al. 1994). The HOTROK code is a computer program that provides an analytical solution of the transient thermal response of a nuclear fuel waste disposal vault (Mathers 1985). The heat sources used in the HOTROK code are cylindrical and uniformly distributed within a semi-infinite rock mass. In the HOTROK model (Baumgartner et al. 1994), the engineered sealing material has the same thermal parameters as the rock.

Figure 41 shows the temperature at panel centre from the Far-Field Model with horizontally finite-dimensional repository and the temperature at repository depth from the Simplified Near-Field Model together with their differences, as computed using COMSOL. For the first one thousand years, there is no difference between two models. At 22,500 years, the difference reaches a peak of 27°C.

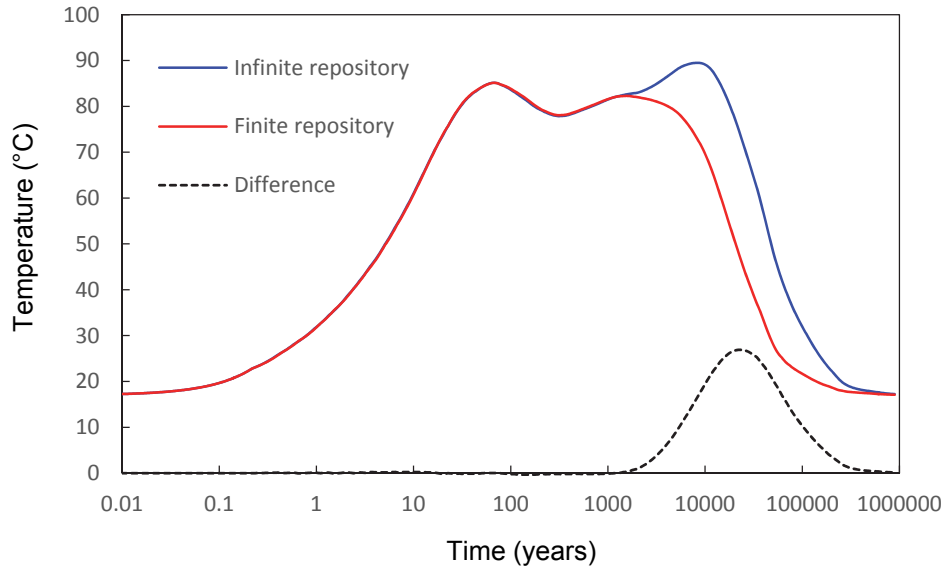


Figure 41: Temperature at Panel Centre from the Far-field Model and Temperature at Repository Depth from the Simplified Near-Field Model and their Differences

Figure 42 shows a comparison of container surface temperatures from the HOTROK model, results from COMSOL model, and modified results from COMSOL model. In the HOTROK model and the COMSOL models, the same thermal parameters as used for the rock are also used for the engineered materials. The container surface temperature from the HOTROK model is an analytical solution, while the COMSOL result is a finite element solution. For the first 1000 years, the results from the COMSOL model match the HOTROK solution well. After 1000 years, the COMSOL model gives a second peak of 88°C at 8,730 years while the HOTROK solution has a second peak of 83°C at 1,000 years. The modified COMSOL result (which is obtained by subtracting the difference shown in Figure 40 from the COMSOL model) matches the HOTROK solution well after 1000 years, thereby providing confidence in the method proposed for accounting for the influence of the adiabatic boundary condition.

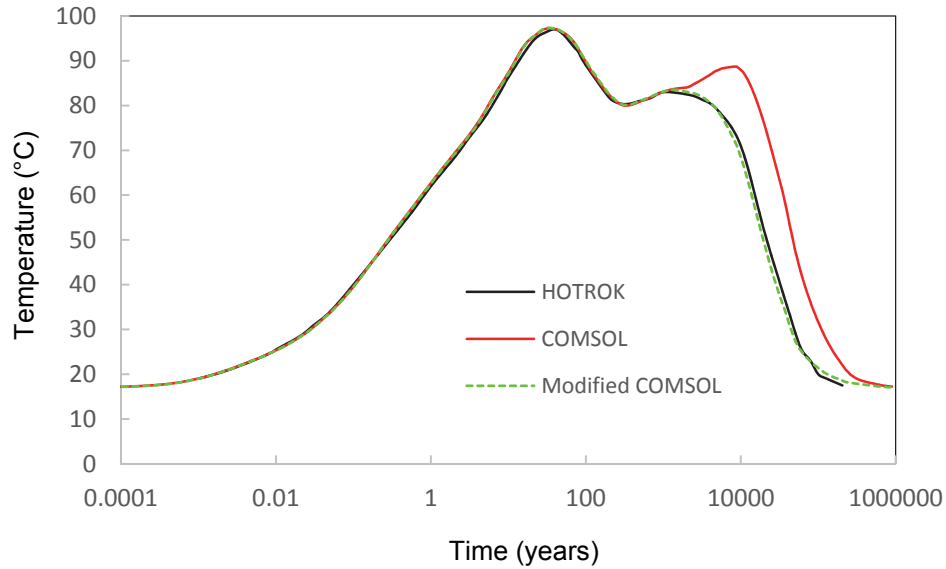


Figure 42: Comparison of Container Surface Temperatures from the HOTROK Model, the Results from COMSOL Model and the Modified Results from COMSOL Model.

8. SUMMARY AND CONCLUSIONS

A series of three-dimensional finite-element thermal-transient analyses has been performed to gain a better understanding of the thermal response in the sealing materials and in the rock for the near-field and far-field areas of a conceptual repository hosted in crystalline rock.

A method is proposed to modify results from the Near-Field Model to account for the effect of applying an adiabatic thermal boundary condition on the four vertical boundaries. The thermal differences between the Far-Field Model and the Simplified Near-Field Model are subtracted from the Near-Field Model results to obtain a more representative thermal response. The modification method is validated by comparing the modified COMSOL results with the HOTROK analytical solution.

A great portion of the temperature change at later times in the non-modified near-field modelling results is attributed to the effect of the adiabatic condition applied on the four vertical boundaries. The modified analysis shows that the thermal peak occurs early in the life of the repository and there is no comparable second peak after thousands of years for the case described in this report.

For the case evaluated, the modified near-field modelling results (i.e., with the effect of the adiabatic boundary condition accounted for) show that the maximum container surface temperature is 84°C occurring at 45 years, the maximum temperature of the room centre between two containers is 83°C occurring at 45 years, and the maximum temperature of the rock at the room roof above the top layer container is 77°C occurring at 65 years.

REFERENCES

- Acres Consulting Services Limited in conjunction with RE/SPEC Ltd. 1985. A feasibility study of the multilevel vault concept. Atomic Energy of Canada Limited Technical Report, TR-297.
- Acres Consulting Services Ltd. 1993. A preliminary study of long-hole emplacement alternatives. Atomic Energy of Canada Limited Technical Report, TR-346.
- Baumgartner, P. 2006. Generic thermal-hydraulic-mechanical (THM) data for sealing materials, Volume 1: soil-water relationship. Ontario Power Generation, Nuclear Waste Management Division 06819-REP-01300-10122-R00.
- Baumgartner, P., T.V. Tran and R. Burgher. 1994. Sensitivity analyses for the thermal response of a nuclear fuel waste disposal vault. Atomic Energy of Canada Limited Technical Report, TR-621, COG-94-258.
- COMSOL. 2015. Heat Transfer Module User's Guide. Version COMSOL. 5.1.
- Golder Associates Ltd. 1993. Used-fuel disposal vault far-field thermal and thermal-mechanical analysis. Atomic Energy of Canada Limited Report, TR-M-015.
- Guo, R. 2007. Numerical modelling of a deep geological repository using the in-floor borehole placement method. Nuclear Waste Management Organization NWMO TR-2007-14. (available at www.nwmo.ca).
- Guo, R. 2008. Sensitivity analyses to investigate the influence of the container spacing and tunnel spacing on the thermal response in a deep geological repository. Nuclear Waste Management Organization NWMO TR-2008-24. (available at www.nwmo.ca).
- Martin, C.D. 1993. The strength of massive Lac du Bonnet granite around underground openings. Ph.D. Thesis, Department of Civil and Geotechnical Engineering, University of Manitoba, Winnipeg, Manitoba, Canada.
- Mathers, W.G. 1985. HOTROK, a program for calculating the transient temperature field from an underground nuclear waste disposal vault. Atomic Energy of Canada Limited Technical Report, TR-366. **
- NWMO. 2005. Choosing a way forward: the future management of Canada's used nuclear fuel. Final study. Nuclear Waste Management Organization report APM-REF-00680-23833 submitted to the Minister, Natural Resource Canada. (Available at www.nwmo.ca).
- Tait, J.C., H. Roman and C.A. Morrison. 2000. Characteristics and radionuclide inventories of used fuel from OPG Nuclear Generating Stations. Volume 1 - Main report; and Volume 2 – Radionuclide inventory data. Ontario Power Generation Report 06819-REP-01200-10029-R00. Toronto, Canada.
- Tsui, K.K. and A. Tsai. 1985. Thermal analyses for different options of nuclear fuel waste placement. Atomic Energy of Canada Limited Report, AECL-7823.