Prediction of the Thermal-Hydraulic-Mechanical Response of a Geological Repository at Large Scale and Sensitivity Analyses – DECOVALEX-2019 Task E: Step 4

NWMO-TR-2019-12

October 2019

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Nuclear Waste Management Organization



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# **Document History**

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#### ABSTRACT

| Title:      | Prediction of the Thermal-hydraulic-mechanical Response of a Geological<br>Repository at Large Scale and Sensitivity Analyses – DECOVALEX-2019<br>Task E: Step 4 |
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#### Abstract

In the current French concept, the High-Level Waste (HLW) will be placed in a set of parallel micro-tunnels 0.75 m to 0.80 m in diameter and 80 m to 150 m length. The HLW zone covers an area of around 8 km<sup>2</sup> in which the rock shows vertical and horizontal mineralogical variation and therefore, the thermal-hydraulic-mechanical (THM) properties are variable. This study presents a case study based on Cigéo data to better assess modelling of deep geological repositories within the DECOVALEX-2019 framework. To gain a better understand the THM response caused by the high-level radioactive waste released heat in the Callovo-Oxfordian formation (COx) for the near field and far-field areas, a series of 2D or 3D coupled THM modelling has been performed.

This work was conducted in the context of the Task E within the DECOVALEX-2019 framework, an international program with a 4-year duration that began in 2016, which is a multidisciplinary, co-operative international research effort in modelling coupled Thermal-Hydraulic-Mechanical-Chemical (THMC) processes in geological systems and addressing their role in Performance Assessment for radioactive waste storage.

In this study, the theory used to perform the coupled THM modelling is validated by comparing the modelled THM results for a point heat source in an infinite rock mass with an analytical solution. The coupled COMSOL model for the case study is also validated by comparing its thermal component for the Base Case with accurate results calculated using other methods.

This study shows that using a 2D model to represent a 3D model has significant influences on the temperature, pore pressure, and stresses at later times and overestimates the ground surface uplift by 64%.

The most important factor influencing temperature development is thermal conductivity. Assuming a minimum value for thermal conductivity results in an overestimate of the temperature at the placement cell centre by 15°C. The most important factor influencing pore pressure is rock permeability. Assuming a minimum rock permeability for COx results in an overestimate of the pore pressure by 28% at the midpoint between two placement cell and 40% near the placement cell. The most important factors influencing the ground surface uplift are rock thermal expansion and rock permeability. The minimum rock thermal expansion could decrease the ground surface uplift estimation by 34%, while the minimum rock thermal expansion could decrease the ground surface uplift estimation by 23%.

The model domain dimensions of 2.0 km x 2.5 km x 3.0 km used based on Cigéo data are sufficiently large such that the bottom hydraulic boundary condition and the thermal/hydraulic boundary condition on the far-field outside vertical surface do not have any obvious influence on the THM modelling results in the centre of the repository.

Assuming the buffer materials in the galleries is fully saturated after 1000 years only slightly influences pore pressure, stresses and ground surface uplift after 1000 years. Assuming the galleries are filled with fully saturated buffer materials can overestimate pore pressure only after 60 years. This does not influence the peak pore pressure but results in an overestimate of the ground surface uplift by 6%.

Applying fixed mechanical boundary condition on the cell wall has a small influence on the horizontal stress perpendicular to the cell axis.

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#### 1. INTRODUCTION

Many countries using nuclear power for the production of electricity, including Canada, are currently considering the long-term disposal of their used nuclear fuel in a deep repository located in a suitable geological formation, such as crystalline rock or sedimentary rock. Geological disposal relies on multiple barriers – for example, engineered clay barriers and thick layers of natural sedimentary rocks – to contain and isolate the radioactive wastes for a very long period of time.

The temperature increase caused by heat input from the used fuel can affect many aspects of near-field and far-field behaviour. For example, the heating and associated temperature variation can change the mechanical behaviour of the rock (Ranjith et al., 2012), and thermal expansion of both the solid rock constituents and the water in the rock pores can create a potential for increased rock damage near the underground openings and progressive rock failure (Read et al., 1998). Rock pore water pressure changes induced by thermal expansion influence both the rock stresses and the hydraulic gradients. Increased pore water pressure in the pores and microfractures of the rock will result in an increase in tensile stress potentially leading to tensile fracturing or causing the hydraulic fracturing to propagate in an unstable manner (Berchenko et al., 1997). Non-uniform pore water pressure increase will alter the existing hydraulic gradients and can affect both the quantity of flow through the rock and the flow direction, thus potentially affecting the advective transport of water-borne radionuclides (Dixon et al., 2002). Therefore, the long-term performance of these barriers is investigated collaboratively by interdisciplinary researchers.

To understand the mechanism of the coupling process, considerable effort has been expended in numerical modelling and interpretation of experiment results related to coupled THM processes (Börgesson and Hernelind, 1999; Rutqvist et al., 2001; Gens et al., 2002; Thomas et al., 2003; Nguyen et al., 2005; Cleall et al., 2006; Guo et al., 2006; Hökmark et al., 2007; Chen and Ledesma, 2009; Gens et al., 2009; Guo, 2011, Bond et al., 2017).

In the current French concept, the High-Level Waste (HLW) will be placed in a set of parallel micro-tunnels 0.75 m to 0.80 m in diameter and 80 m to 150 m length as shown in Figure 1. The HLW zone covers an area of around 8 km<sup>2</sup> of the geological formation of the Callovo-Oxfordian (COx) in which the rock shows vertical and horizontal mineralogical variation and therefore, the thermal-hydraulic-mechanical (THM) properties are variable. COx sediments comprise a dominant clay fraction rich in carbonates, guartz, minor feldspars and accessory minerals. On an average, the COx contains 25-55% clay minerals, 20-38% carbonates, 20-30% quartz, 1% feldspar, and small amount of others (Andra, 2005). The sedimentation has caused a preferential orientation of the clay foliage and consequently a stratification of the matrix structure. This consequently results in anisotropy of the rock properties. An anisotropic behaviour is found in the COx based on the mechanical tests performed on the samples obtained following different orientations. The parallel to bedding stiffness of the COx is greater than its perpendicular to bedding stiffness. Horizontal thermal conductivity (i.e., parallel to the bedding) of the COx is also higher than the vertical one. Concerning the water permeability, a slight anisotropy ratio between 2 and 3 is observed (Armand et al., 2017b). An anisotropic in situ initial stress is also observed (Armand et al., 2017b). The largest principal stress is horizontal, and the vertical stress and the smallest horizontal stress are similar in magnitude (Wileveau et al., 2007). At the main level of the URL (i.e., at -490 m) the maximum stress, which is parallel to the direction of the heater boreholes, is about 16 MPa and both the middle and the minor stresses are about 12 MPa (Armand et al., 2017b). The hydraulic and mechanical response is also influenced by the orientation of the initial in situ stress directions (Armand et al., 2013, 2014, 2017a, 2017b).



Figure 1: Diagram of the Facilities of the Cigéo project<sup>1</sup>

To gain a better understanding the THM response caused by the radioactive waste released heat in the COx for the near field and far-field areas of the HLW cells, a series of 2D or 3D coupled THM modelling has been performed. The current study has been conducted in Task E within the DECOVALEX-2019 framework, an international program with a 4-year duration that began in 2016. DECOVALEX is a multidisciplinary, co-operative international research effort in modelling coupled Thermal-Hydraulic-Mechanical-Chemical (THMC) processes in geological systems and addressing their role in Performance Assessment for radioactive waste storage (Stephansson et al., 2004). The project deals with several processes of importance for radioactive release and transport. Fourteen funding organizations from industry and regulatory authorities have participated to date in one or more modelling tasks of the project. The primary purpose of Task E is to upscale THM modelling from small size experiments (some cubic meters) to real scale cell (some ten cubic meters) and to scale of the waste repository (cubic kilometers) (Seyedi et al., 2019). The Nuclear Waste Management Organization (NWMO) is one of the funding organizations of DECOVALEX-2019 and participates in the modelling activity of Task E. The goal of Task E is to propose guidelines for repository-scale calculations for a deep repository in COx claystone by assessing the effect of choice of THM modelling. Some data are coming from the Cigéo project but are just used as a case study. Calculation presented in the following section are not part of the design of the real project.

This report describes the work completed in support of Step 4 of the DECOVALEX-2019 Task E by NWMO.

<sup>&</sup>lt;sup>1</sup> From DECOVALEX-2019 7<sup>th</sup> workshop's presentation of "Task E: Synthesis and discussions" authored by Armand G., Plua C. and Vu M.-N.

# 2. AIM OF THE DECOVALEX-2019 TASK E STEP 4

The main objective of Step 4 of the DECOVALEX-2019 Task E is to investigate how to make reliable numerical modelling at the repository scale regarding the variability of THM parameters on such a scale (Seyedi et al., 2020).

To assess the influence of the variability of THM parameters on the THM response of the COx in terms of the temperature, pore water pressure and effective stress evolution, the following studies are performed:

- Studies using a coupled THM 3-dimensional model, which is one quarter of the HLW repository, and a 2-dimension model, using mean values of THM parameters,
- Sensitivity studies on the THM parameters of the COx,
- Sensitivity studies on the THM parameters in the layer above or below the layer containing the repository,
- Model reliability studies on boundary conditions, model dimension and model simplification, and
- Model validation studies.

## 3. COUPLED THM COMSOL THEORETICAL MODEL

Figure 2 illustrates the coupled effects. Temperature changes can affect the fluid flow and mechanical response, and mechanical response can affect fluid flow. Changes in temperature develop thermal stresses in the rock and the changes in stresses and strains alter rock porosity and progressively alter rock strength, thereby affecting hydraulic permeability and altering pore water pressure. In turn, thermally induced stresses in the rock also change the hydraulic flow, which, therefore, changes the thermal advection. Fluid flow in the rock pores can affect the effective stresses in the rock through the pore water pressure. The hydraulic properties (fluid density, viscosity and porosity) are also affected by the variation in temperature and change the pore water pressure.



Figure 2: A THM Coupling Flowchart

COMSOL Multiphysics v5.4 is used to perform this modelling exercise. COMSOL Multiphysics is a finite element modelling environment used to model and solve all kinds of scientific and engineering problems. The software provides an integrated desktop environment with a Model Builder that allows the user to solve coupled physics phenomena (COMSOL, 2018a, 2018b).

#### 3.1 THERMAL EQUATIONS

The following thermal equation is used for thermal modelling (COMSOL, 2018a):

$$c_p \rho \frac{\partial T}{\partial t} + \rho_w c_{pw} \nu \nabla T + \nabla q = Q$$
<sup>(1)</sup>

where *T* is temperature (K), *t* is time (s),  $\rho$  is bulk density (kg/m<sup>3</sup>),  $c_p$  is specific heat capacity of the porous matrix (J/(kg·K)), *Q* is a specific source of heat (W/m<sup>3</sup>),  $\rho_w$  is the density of water (kg/m<sup>3</sup>),  $c_{pw}$  is specific heat capacity of water (J/(kg·K)), *v* is Darcy's velocity (m/s), and *q* is the heat flux (W/m<sup>2</sup>), which can be defined as follows (COMSOL, 2018a):

$$q = -\lambda \nabla T \tag{2}$$

where  $\lambda$  is the thermal conductivity tensor (W/(m·K)).

#### 3.2 HYDRAULIC EQUATIONS

Water balance equation is used for the coupled model as follows:

$$\frac{\partial(\phi\rho_w)}{\partial t} + \phi\rho_w \frac{1}{1+\varepsilon_v} \frac{\partial\varepsilon_v}{\partial t} - \nabla\left(\rho_w \frac{k}{\mu}\nabla(p-\rho_w gz)\right) = 0$$
(3)

where *p* is water pressure (Pa), *g* is the vector of gravity (m/s<sup>2</sup>), *z* is the vertical coordinate (m), *k* is permeability (m<sup>2</sup>),  $\varepsilon_v$  is the volumetric strain (unitless),  $\mu$  is viscosity (Pa s), which is a function of temperature and can be expressed as follows (Andrade, 1930):

$$\mu = Aexp(\frac{B}{r}) \tag{4}$$

where A is pre-exponential parameter (Pa s), B is exponential parameter (K).

 $\phi$  is porosity (unitless), which is a function of temperature and volumetric strain and can be expressed as follows:

$$\phi = (\phi_0 + \alpha_B \varepsilon_v + (\alpha_B - \phi_0)(p - p_0)(1 - \alpha_B)C_m - \alpha_s(\alpha_B - \phi_0)(T - T_0))/(1 + \varepsilon_v)$$
(5)

where  $\alpha_s$  is the volumetric thermal expansion of the rock (1/K),  $\phi_0$  is the initial porosity (unitless),  $C_m$  is the compressibility of the solid phase (Pa<sup>-1</sup>),  $\alpha_B$  is the Biot coefficient (unitless),  $\varepsilon_v$  is the volumetric strain (unitless),  $p_0$  is the reference pressure (Pa), and  $T_0$  is the reference temperature (K).

 $\rho_w$  is the density of water (kg/m<sup>3</sup>),  $\rho_w$  is a function of temperature and pore pressure and can be linearly expressed as follows (Muller et al., 1981):

$$\rho_w = \rho_0 (1 + \beta (p - p_0) - \alpha_w (T - T_0))$$
(6)

where  $\rho_0$  is the density of water at reference pressure and reference temperature (kg/m<sup>3</sup>),  $\beta$  is the water compressibility (1/Pa), and  $\alpha_w$  is the water volumetric thermal expansion coefficient (1/K).

#### 3.3 MECHANICAL EQUATIONS

In this exercise, the COx is assumed to be an elastic material. The following equation is used for the mechanical response of the COx, including hydraulic and thermal effects (COMSOL, 2018b):

$$\rho \frac{\partial^2 \boldsymbol{u}}{\partial t^2} - \nabla \cdot \overline{\boldsymbol{S}} = \boldsymbol{F}_{\boldsymbol{v}} \tag{7}$$

where  $\boldsymbol{u}$  is the deformation vector,  $\boldsymbol{F}_{v}$  is the volume force,  $\overline{\boldsymbol{S}}$  is the effective stress increase tensor and is equal to  $\overline{\boldsymbol{\sigma}} - \overline{\boldsymbol{\sigma}}_{0} - \alpha_{B}(p - p_{0})\overline{\boldsymbol{I}}$ ,  $\overline{\boldsymbol{\sigma}}$  is the total stress tensor.

$$\overline{\boldsymbol{\sigma}} - \overline{\boldsymbol{\sigma}}_0 - \alpha_B (p - p_0) \overline{\boldsymbol{I}} = \overline{\boldsymbol{C}} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_T)$$
(8)

where  $\overline{\sigma}_0$  is the initial stress tensor, p is the pore water pressure calculated from the hydraulic model,  $\overline{I}$  is a 3x3 identity matrix,  $\varepsilon$  is the strain tensor,  $\varepsilon_0$  is the initial strain tensor,  $\overline{C}$  is the 4<sup>th</sup> order elasticity tensor, ":" stands for the double-dot tensor product (or double contraction), and  $\varepsilon_T$  is the strain due to thermal expansion and can be calculated using the following equation:

$$\boldsymbol{\varepsilon}_T = \frac{\alpha_s}{3} (T - T_0) \boldsymbol{\overline{I}} \tag{9}$$

The strain is calculated using the following equation:

$$\boldsymbol{\varepsilon} = \frac{1}{2} \left[ (\nabla \boldsymbol{u})^T + \nabla \boldsymbol{u} \right] \tag{10}$$

## 4. COUPLED THM COMSOL MODEL

# 4.1 GEOMETRY AND MESH DISCRETIZATION

Figure 3 shows the geometry of the COMSOL model of the Base Case for the coupled thermohydro-mechanical simulation of a deep geological repository in the COx in France. The model geometry dimensions are 2 km x 2.5 km x 3.0 km. It includes 3 access galleries and one connection gallery. There are total 168 cells modelled, in which 162 cells were represented using cuboid blocks and six cells are modelled in detail with individual tunnels resolved in the model (L1 to L6 as shown in Figure 3 and Figure 4).

There are eight layers of geological units considered in this model. The depths of the different geological units are shown in Table 1.

|                   | Formation        | Depth (m)                                  | Thickness (m) |
|-------------------|------------------|--|---------------|
| Barrois Limestone |                  | 0 – 103.4                                  | 103.4         |
|                   | Kimmeridgian     | 103.4 – 211.4                              | 108           |
| Carb              | onated Oxfordian | 211.4 – 488.0                              | 276.6         |
| Callovo-Oxfordian | USC              | 488.0 – 517.4                              | 29.4          |
|                   | UT               | 517.4 – 532.6                              | 15.2          |
|                   | UA23 (UA2-UA3)   | 532.6 – 595.8<br>(cells at depth of 560 m) | 63.2          |
|                   | UA1              | 595.8– 635.0                               | 39.2          |
| Dogg              | er               | >635.0                                     |               |

# Table 1: Depths of Each Geological Unit considered in the COMSOL Model and its Thickness

Modelling results are provided at four locations, which are represented as Points P1, P2, P3 and P4 shown in Figure 3 and Figure 4. P1 (Px/2, Px is the cell spacing) is centrally located between Cell L3 and Cell L4. P2 is the centre of Cell L3, P3 is 2 m ( $2.5\Phi_{cell}$ ) far from Point P2 and P4 is on the ground surface above P1.

- The temperature, pore pressure and stresses are calculated at Points P1 and P3;
- The temperature is calculated at Point P2; and
- The uplift is calculated at Point P4.

Figure 5 shows the mesh of the THM COMSOL model. There are 168,785 tetrahedral elements and 229,223 nodes. The maximum and minimum sizes in the formation of the UA2 – UA3 (UA23) layer are 200 m and 0.616 m respectively.



Figure 3: Model Geometry with Details of 6 Placement Cells of the Base Case



Figure 4: Local Details of Placement Cells and Points for Output near the Placement Cells



Figure 5: Mesh for the THM COMSOL Model of the Base Case

# 4.2 INITIAL AND BOUNDARY CONDITIONS FOR THE BASE CASE

## 4.2.1 Initial Conditions for the Base Case

The excavation of the access tunnels and connection tunnel is simulated and the THM results from the simulation of the access and connection tunnels are considered as the initial conditions for the cell excavation and heating stage. The time between the access tunnel / connection tunnel excavation and the cell excavation is fixed to 10 years. The cell excavation occurs at Year 0. The HLW packages are placed inside the cells two years later.

The initial temperature for the simulation of excavation of the access/connection tunnels is a function of depth from the ground surface as shown in Figure 6.



Figure 6: Initial Temperature in Entire Model for Simulation of Access/Connection Tunnel Excavation

The initial pore water pressure for simulation of excavation of the access/connection tunnels is a function of the depth as follows:

$$p_0 = 0.1 MPa + 0.0098 MPa/m \times z \tag{11}$$

in which z is the depth from the ground surface, m.

The initial stresses for the simulation of the excavation of the access/connection tunnels are shown in Figure 7.



Figure 7: Initial Stresses in Entire Model for Simulation of Access/Connection Tunnel Excavation

#### 4.2.2 Boundary Conditions for the Base Case

The temperature on the top surface (Plane O'A'B'C'), the bottom surface (Plane OABC), the back surface (Plane CBB'C') and the right surface (Plane AA'B'B) is also a function of depth from the ground surface as shown in Figure 6. Adiabatic condition is applied on the left surface (Plane OO'C'C) and the front surface (Plane OO'A'A) (assuming they are symmetric surfaces). The heat power per meter cell as a function of time is shown in Figure 8.



Figure 8: Heat Power per Meter Cell with Time

The pore pressure on the top surface, the bottom surface, the back surface (Plane BB'C'C) and the right surface (Plane AA'B'B) is a function of depth from the ground surface as shown in Equation (11). No hydraulic flow is assumed to cross the left surface and the front surface (assuming they are symmetric surfaces).

The top surface is a mechanical free surface. A normal stress  $s_{xx}$  which is a function of depth as shown in Figure 7 is applied on the right surface. A normal stress  $s_{yy}$  which is also a function of depth as shown in Figure 7 is applied on the back surface. A roller boundary condition is applied on the left, front and bottom surface.

Boundary conditions of the cells and the access tunnel during the two stages of the simulations are shown in Table 2, and have been defined by DECOVALEX-2019 Task E.

| Time               | Boundary<br>Type | Cells  | Access tunnel        |
|--------------------|------------------|--|----------------------|
|                    | Thermal          | Initial temperature                          | Initial temperature  |
| 0 – 2 years        | Hydraulic        | draulic Atmospheric pressure Atmospheric pre |                      |
|                    | Mechanical       | Free surface                                 | Free surface         |
| 0 40000            | Thermal          | Heat power                                   | No flux              |
| 2 – 10000<br>years | Hydraulic        | No flux                                      | Atmospheric pressure |
|                    | Mechanical       | Free surface                                 | Free surface         |

 Table 2: Boundary Conditions on the Cell and Tunnel Walls for the Base Case

# 4.3 MATERIAL PARAMETERS

Table 3 shows the values of the THM parameters of each layer in the vertical direction used for the simulation in the Base Case and these parameters are defined by DECOVALEX-2019 Task E. Table 4 shows the ratios of each parameter in the horizontal direction against its corresponding value in the vertical direction and they are defined by DECOVALEX-2019 Task E. In Tables 4, 5, 8 and 9, the following terms are used to stand for:

Geological formation terms:

- bar Barrois limestone,
- Kim Kimmeridgian,
- Oxf –Carbonated Oxfordian,
- usc COx USC,
- ut COx UT,
- ua23 COx UA2-UA3,
- ua1 COx UA1, and
- dog Dogger.

Parameter terms:

- Ey\_v vertical Young's modulus,
- nu\_hv vertical Poisson's ratio,
- biot Biot coefficient,
- n0 initial porosity,
- kw\_v vertical permeability,
- rhoeq equivalent density,
- Imbp\_v thermal conductivity,
- alphas linear thermal expansion, and
- Cp thermal capacity,

|      | Ey_v<br>[Pa] | nu_hv  | biot   | n0      | kw_v<br>[m²] | rhoeq<br>[kg/m³] | lmbp_v<br>[W/(m K)] | alphas<br>[K <sup>-1</sup> ] | Cp<br>[J/(kg K)] |
|------|--------------|--------|--------|---------|--------------|------------------|---------------------|------------------------------|------------------|
| bar  | 3.60E+09     | 3.0E-1 | 6.0E-1 | 1.30E-1 | 1.00E-19     | 2.45E+03         | 1.10E+00            | 2.20E-05                     | 1.024E+03        |
| Kim  | 3.60E+09     | 3.0E-1 | 6.0E-1 | 1.30E-1 | 1.00E-19     | 2.45E+03         | 1.10E+00            | 2.20E-05                     | 1.024E+03        |
| Oxf  | 3.00E+10     | 3.0E-1 | 6.0E-1 | 1.30E-1 | 1.00E-16     | 2.47E+03         | 2.30E+00            | 4.50E-06                     | 9.250E+02        |
| usc  | 1.28E+10     | 3.0E-1 | 6.0E-1 | 1.50E-1 | 1.87E-20     | 2.48E+03         | 1.79E+00            | 1.75E-05                     | 9.780E+02        |
| ut   | 8.50E+09     | 3.0E-1 | 6.0E-1 | 1.73E-1 | 1.87E-20     | 2.45E+03         | 1.47E+00            | 1.75E-05                     | 9.780E+02        |
| ua23 | 7.00E+09     | 3.0E-1 | 6.0E-1 | 1.93E-1 | 1.87E-20     | 2.42E+03         | 1.31E+00            | 1.75E-05                     | 9.780E+02        |
| ua1  | 1.25E+10     | 3.0E-1 | 6.0E-1 | 1.64E-1 | 1.87E-20     | 2.46E+03         | 1.63E+00            | 1.75E-05                     | 9.780E+02        |
| dog  | 3.00E+10     | 3.0E-1 | 6.0E-1 | 1.00E-1 | 1.00E-18     | 2.47E+03         | 2.30E+00            | 4.50E-06                     | 9.250E+02        |

Table 3: THM Parameters for the Base Case

Table 4: Anisotropy Ratios of the THM Parameters

|      | Ey_r     | nu_r     | kw_r     | lmbp_r   |
|------|----------|----------|----------|----------|
| bar  | 1.00E+00 | 1.00E+00 | 1.00E+00 | 1.40E+00 |
| kim  | 1.00E+00 | 1.00E+00 | 1.00E+00 | 1.40E+00 |
| oxf  | 1.00E+00 | 1.00E+00 | 1.00E+00 | 1.00E+00 |
| usc  | 1.50E+00 | 1.00E+00 | 3.00E+00 | 1.00E+00 |
| ut   | 1.50E+00 | 1.00E+00 | 3.00E+00 | 1.50E+00 |
| ua23 | 1.50E+00 | 1.00E+00 | 3.00E+00 | 1.50E+00 |
| ua1  | 1.50E+00 | 1.00E+00 | 3.00E+00 | 1.50E+00 |
| dog  | 1.00E+00 | 1.00E+00 | 1.00E+00 | 1.00E+00 |

Water parameters used in these models are shown in Table 5. Dynamic viscosity of water is a function of temperature as shown in Equation (4).

| Parameters   | Water  |
|--|--|
| Reference density of water (kg/m <sup>3</sup> )      | 1000   |
| Compressibility of water (1/Pa)                      | 4.0x10 <sup>-10</sup>                            |
| Heat capacity of water (J/(kg <sup>-</sup> K))       | 4180   |
| Dynamia viscosity of water (Baja)                    | A = 2.1x10 <sup>-6</sup> (Pa <sup>-</sup> s) and |
| Dynamic viscosity of water (Pa's)                    | <i>B</i> = 1808.5 (K)                            |
| Water volumetric thermal expansion coefficient (1/K) | $\alpha_w(T)$ as shown in Figure 9               |



Figure 9: Water Volumetric Thermal Expansion Coefficient

When the sensitivity cases regarding the gallery wall boundary conditions are studied, the galleries are filled with buffer materials at a certain time (e.g., at 2 years or at 1000 years). The THM parameters for buffer materials are shown in Table 6.

| Parameters                              | Value               |
|---|---------------------|
| Young's modulus (MPa)                   | 300                 |
| Poisson's ratio                         | 0.3                 |
| Thermal conductivity (W/m/K)            | 1.79                |
| Porosity                                | 0.3                 |
| Volumetric thermal expansion (1/K)      | 5.25x10⁻⁵           |
| Thermal specific heat capacity (J/kg/K) | 978                 |
| Permeability (m <sup>2</sup> )          | 5x10 <sup>-21</sup> |
| Equivalent density (kg/m <sup>3</sup> ) | 2465                |

| <b>Table 6: Buffer Material T</b> | <b>FHM Parameters</b> |
|-----------------------------------|-----------------------|
|-----------------------------------|-----------------------|

When sensitivity cases examining the cell wall boundary condition are studied, the material properties of the cells are assumed to be those of steel. The THM parameters for steel are shown in Table 7.

| Parameters   | Value              |  |
|--|--------------------|--|
| Young's modulus (MPa)  | 20000 <sup>*</sup> |  |
| Poisson's ratio  | 0.2*               |  |
| Thermal conductivity (W/m/K)   | 40*                |  |
| Volumetric thermal expansion (1/K)                                   | 0                  |  |
| Thermal specific heat capacity (J/kg/K)                              | 430*               |  |
| Equivalent density (kg/m <sup>3</sup> )                              | 2465               |  |
| * From Engineering Teelbox at website of your Engineeringteelbox com |                    |  |

**Table 7: Steel Cell Material Thermal and Mechanical Parameters** 

From Engineering Toolbox at website of www.Engineeringtoolbox.com

# 5. BASE CASE MODELLING RESULTS

This section describes the modelling results related to the Base Case. For the Base Case, the mean values of the THM parameters are used except for the Biot coefficient for which the minimum value (0.6) is used.

# 5.1 TEMPERATURE AT CELL CENTRE, 2.5 $\phi_{cell}$ AND PX/2

Figure 10 shows the temperature at Cell centre,  $2.5\phi_{cell}$  and Px/2. The peak temperature at cell centre (P2),  $2.5\phi_{cell}$  (P3), and Px/2 (P1) are 75.8°C after 11.8 years, 59°C after 29.7 years and 44°C after 387 years, respectively.



Figure 10: Simulated Temperatures at Points P1 (Px/2), P2 (cell centre) and P3 (2.5Φcell)

# 5.2 PRESSURE AT 2.5 $\phi_{cell}$ AND PX/2

Figure 11 shows the simulated pore pressures at Points  $2.5\phi_{cell}$ , and Px/2 with time. The peak pore pressures are 12.0 MPa at Point  $2.5\phi_{cell}$  after 40 years and 12.3 MPa at Point Px/2 after 38 years.



Figure 11: Simulated Pore Pressure at Points P1 (Px/2) and P3 (2.5Φcell)

#### 5.3 MECHANICAL RESPONSE

# 5.3.1 Biot Effective Stress at $2.5\phi_{cell}$ and Px/2

Biot effective stress is calculated using the following equation:

$$\sigma' = \sigma - \alpha_B \cdot p \tag{12}$$

in which  $\sigma'$  is Biot effective stress.

Figure 12 shows the simulated X-directional stress at Points  $2.5\phi_{cell}$ , and Px/2 with time. The peak stresses are 17.9 MPa at Point  $2.5\phi_{cell}$  after 35 years and 18.2 MPa at Point Px/2 after 680 years.



Figure 12: Simulated Stress in the X-direction at Points  $2.5\phi_{cell}$  and Px/2 from the Base Case Study

Figure 13 shows the simulated Y-directional stress at Points  $2.5\phi_{cell}$ , and Px/2 with time. The peak stresses are 24.2 MPa at Point  $2.5\phi_{cell}$  after 15 years and 21.9 MPa at Point Px/2 after 820 years.



Figure 13: Simulated Stress in the Y-direction at Points  $2.5\phi_{cell}$  and Px/2 from the Base Case Study

Figure 14 shows the simulated Z-directional stress at Points  $2.5\phi_{cell}$ , and Px/2 with time. The lowest stresses are 12.2 MPa at Point  $2.5\phi_{cell}$  after 85 years and 9.9 MPa at Point Px/2 after 32 years.



Figure 14: Simulated Stress in the Z-direction at Points 2.5 $\phi_{cell}$  and Px/2 from the Base Case Study

#### 5.3.2 Vertical Displacement on the Surface

Figure 15 shows the simulated uplift at Point P4 with time. The peak value of uplift is 9.3 cm after 1570 years.



Figure 15: Simulated Uplift at P4 (ground surface above P2) from the Base Case Study

In summary, the temperatures reach peak values of 75.8°C at the cell centre 11.8 years after gallery excavation, 59°C at Point  $2.5\Phi_{cell}$  at Year 29.7, and 44°C at mid-point (Px/2) between two cells at Year 387. The pore pressures are 12.0 MPa at Point  $2.5\Phi_{cell}$  after 40 years and 12.3 MPa at Point Px/2 after 38 years. The peak X-directional stresses are 17.9 MPa at Point  $2.5\Phi_{cell}$  after 35 years and 18.2 MPa at Point Px/2 after 680 years. The peak Y-directional stresses are 24.2 MPa at Point  $2.5\Phi_{cell}$  after 15 years and 21.9 MPa at Point Px/2 after 820 years. The lowest Z-directional stresses are 12.2 MPa at Point  $2.5\Phi_{cell}$  after 85 years and 9.9 MPa at Point Px/2 after 31.6 years. The simulated uplift on the ground surface above the panel centre reaches its peak value of 9.6 cm after 1570 years.

## 6. SENSITIVITY ANALYSES

In this section, the following studies were performed:

- Comparison of the analysis between the 2D model and the 3D model,
- Parameter analysis,
- Boundary conditions,
- Influence of model simplification,
- Influence of model vertical size, and
- Influence of modelling 4 panels instead of 6 panels

# 6.1 COMPARISON ANALYSIS BETWEEN 2D MODEL AND 3D MODEL

Coupled THM 3D modelling typically requires significant computational resources and execution time. There is a desire to see if a 2D model can be used (instead of a 3D model) to accurately represent the THM response of a deep geological repository. An analysis is performed using 2D version of the Base Case model in which parameters used are the same as those used in the 3D Base Case model. Results from the 2D Base Case model are compared with the results from the 3D Base Case model.

Figure 16 shows the two-dimensional model geometry. It is a vertical cross-section of the 3D model shown in Figure 3 through Points P1, P2, P3 and P4. It models 28 placement cells. Twenty two cells are represented using two rectangles (each representing 11 cells). The central 6 placement cells are represented in detail as in the 3D model. The model dimensions are 2.5 km x 3.0 km.

Figure 17 shows the mesh used for the 2D COMSOL model. It contains 15,160 triangular elements and 24,031 nodes.



Figure 16: Two-Dimension Model Geometry



Figure 17: Mesh for Two-Dimension Model Geometry

Figure 18 shows the temperature comparison between 2D model and 3D model at locations of Points P1, P2 and P3. There is no obvious difference between the 2D model and 3D model during the first 100 heating years. After 100 years, the 2D model overestimated the temperatures at different locations. The maximum observed difference between the 2D and 3D models was 3°C and occurred at 700 years.



Figure 18: Comparison of Temperature from 2-Dimensional and 3-Dimensional Models for Base Cases at Points P2 (Cell centre), P3 ( $2.5\phi_{cell}$ ) and P1 (Px/2).

Figure 19 shows the comparison of the pore water pressure between the 2D model and 3D model at Points P1 and P3. There is no differences in pore water pressure during the first 40 years. After 40 years the 2D model greatly overestimated the pore water pressure. The maximum observed difference between the 2D and 3D models was 3.7 MPa (51%) and occurred at 500 years. However, the difference between the maximum values obtained with 3D and 2D models reduces to a 13.8 % (i.e., (14 MPa-12.3 MPa)/12.3 MPa).



Figure 19: Comparison of Pore Pressure from 2-Dimensional and 3-Dimensional Models for Base Cases at Points P1 (Px/2) and P3 ( $2.5\phi_{cell}$ )

Figures 20, 21 and 22 show the comparison of the X-directional, Y-directional and Z-directional stresses at Points P1 and P3 between the 2D model and the 3D model. For the first two years (before heating), the 2D model overestimated the X-directional stress at Point P3. For the first 10 heating years, there is no obvious difference of the X-directional effective stress at both locations. After 40 years of heating, the effective X-directional stress at P1 and P3 both were underestimated by the 2D model because of the overestimation of the pore water pressure. Only small differences were observed in the stress in the Y-direction.



Figure 20: Comparison of Stress in the X-Direction from 2-Dimensional and 3-Dimensional Models for Base Cases at Points P1 (Px/2) and P3 ( $2.5\phi_{cell}$ )


Figure 21: Comparison of Stress in the Y-Direction from 2-Dimensional and 3-Dimensional Models for Base Cases at Points P1 (Px/2) and P3 ( $2.5\phi_{cell}$ )

For the Z-directional stress, the effective stress at Point P1 decreases to a minimum value of 9.9 MPa at 31.6 years from the 3D model while its minimum value is 8.3 MPa at 80 years from the 2D model. At Point P3, the minimum value of the 3D model is 12.2 MPa at 85 years while the minimum value of the 2D model is only 9.5 MPa at 163 years.



Figure 22: Comparison of Stress in the Z-Direction from 2-Dimensional and 3-Dimensional Models for Base Cases at Points P1 (Px/2) and P3 ( $2.5\phi_{cell}$ )

Figure 23 shows the comparison of the uplift at Point P4 between the 2D and 3D models. The 2D model greatly overestimates the uplift at the ground surface (P4). The peak value is 15.7 cm from the 2D model against 9.6 cm from the 3D model (an increase of 64%). The reason is that the heat load beyond the range of the repository in the Y-direction, which does not exist in reality but does in the 2D model, causes additional uplift on the ground surface.



#### Figure 23: Comparison of Uplift from 2-Dimensional and 3-Dimensional Models for Base Cases at Point P4 which is on the Ground Surface above Point 2

In summary, the 2D model significantly overestimates the THM response of a deep geological repository. The thermal results between the 2D and 3D models were found to have the best agreement within the first 100 years, the hydraulic results had good agreement within the first 40 years, and the mechanical results had good agreement within the first 40 years. Maximum observed differences between the 2D and 3D model were found to be 7% for temperature, 51% for pore pressure and 64% for surface uplift.

### 6.2 SENSITIVITY ANALYSES OF THM PARAMETER USING 3D MODEL

In this section, the influence of the different THM parameters on the THM responses is studied. It includes the influence of the minimum or maximum values of each THM parameter used for all layers of USC, UT, UA23 and UA1, the minimum or the maximum values of hydraulic permeability of each layer, the minimum or the maximum values of thermal conductivity for Layer USC or for Layer UT, and the minimum or the maximum values of Young's modulus of Layer USC.

### 6.2.1 Analyses of Parameters of Layers USC, UT, UA23 and UA1

Tables 8 and 9 show the minimum values or maximum values of the THM parameters used for different units of rock in the COMSOL model and these values are defined by DECOVALEX-2019 Task E.

|      | Ey_v [Pa] | nu_hv  | biot   | n0      | kw_v [m²] | rhoeq [kg/m <sup>3</sup> ] | lmbp_v<br>[W/(m K)] | alphas [K <sup>-1</sup> ] | Cp [J/(kg K)] |
|------|-----------|--------|--------|---------|-----------|----------------------------|---------------------|---------------------------|---------------|
| bar  | 3.60E+09  | 3.0E-1 | 6.0E-1 | 1.30E-1 | 1.00E-19  | 2.45E+03                   | 1.10E+00            | 2.20E-05                  | 1.024E+03     |
| Kim  | 3.60E+09  | 3.0E-1 | 6.0E-1 | 1.30E-1 | 1.00E-19  | 2.45E+03                   | 1.10E+00            | 2.20E-05                  | 1.024E+03     |
| Oxf  | 3.00E+10  | 3.0E-1 | 6.0E-1 | 1.30E-1 | 1.00E-16  | 2.47E+03                   | 2.30E+00            | 4.50E-06                  | 9.250E+02     |
| usc  | 5.50E+09  | 2.0E-1 | 6.0E-1 | 9.70E-2 | 2.60E-21  | 2.42E+03                   | 1.29E+00            | 1.00E-05                  | 8.420E+02     |
| ut   | 4.00E+09  | 2.0E-1 | 6.0E-1 | 1.43E-1 | 2.60E-21  | 2.40E+03                   | 1.08E+00            | 1.00E-05                  | 8.420E+02     |
| ua23 | 3.70E+09  | 2.0E-1 | 6.0E-1 | 1.50E-1 | 2.60E-21  | 2.34E+03                   | 9.80E-01            | 1.00E-05                  | 8.420E+02     |
| ua1  | 3.80E+09  | 2.0E-1 | 6.0E-1 | 1.28E-1 | 2.60E-21  | 2.40E+03                   | 1.12E+00            | 1.00E-05                  | 8.420E+02     |
| dog  | 3.00E+10  | 3.0E-1 | 6.0E-1 | 1.00E-1 | 1.00E-18  | 2.47E+03                   | 2.30E+00            | 4.50E-06                  | 9.250E+02     |

Table 8: Minimum Values of THM Parameters

Table 9: Maximum Values of THM parameters

|      | Ey_v [Pa] | nu_hv  | biot    | n0      | kw_v [m²] | rhoeq<br>[kg/m <sup>3</sup> ] | lmbp_v<br>[W/(m K)] | alphas [K <sup>-1</sup> ] | Cp [J/(kg K)] |
|------|-----------|--------|---------|---------|-----------|-------------------------------|---------------------|---------------------------|---------------|
| bar  | 3.60E+09  | 3.0E-1 | 6.0E-01 | 1.30E-1 | 1.00E-19  | 2.45E+03                      | 1.10E+00            | 2.20E-05                  | 1.024E+03     |
| Kim  | 3.60E+09  | 3.0E-1 | 6.0E-01 | 1.30E-1 | 1.00E-19  | 2.45E+03                      | 1.10E+00            | 2.20E-05                  | 1.024E+03     |
| Oxf  | 3.00E+10  | 3.0E-1 | 6.0E-01 | 1.30E-1 | 1.00E-16  | 2.47E+03                      | 2.30E+00            | 4.50E-06                  | 9.250E+02     |
| usc  | 2.01E+10  | 4.0E-1 | 1.0E+00 | 1.85E-1 | 7.33E-20  | 2.54E+03                      | 2.45E+00            | 2.50E-05                  | 1.114E+03     |
| ut   | 1.28E+10  | 4.0E-1 | 1.0E+00 | 2.06E-1 | 7.33E-20  | 2.49E+03                      | 1.91E+00            | 2.50E-05                  | 1.114E+03     |
| ua23 | 1.07E+10  | 4.0E-1 | 1.0E+00 | 2.49E-1 | 7.33E-20  | 2.48E+03                      | 1.81E+00            | 2.50E-05                  | 1.114E+03     |
| ua1  | 2.18E+10  | 4.0E-1 | 1.0E+00 | 2.05E-1 | 7.33E-20  | 2.51E+03                      | 2.22E+00            | 2.50E-05                  | 1.114E+03     |
| dog  | 3.00E+10  | 3.0E-1 | 6.0E-01 | 1.00E-1 | 1.00E-18  | 2.47E+03                      | 2.30E+00            | 4.50E-06                  | 9.250E+02     |

Figures 24, 25 and 26 show the influence of the thermal conductivity, specific heat capacity, and equivalent density of rock of Layers USC, UT, UA23 and UA1 on the temperature at P1, P2 and P3. The sequence of parameters with greatest to least influence on temperature is:

Thermal conductivity > Specific heat capacity > Equivalent density.

The minimum values of thermal conductivity of Layers USC, UT, UA23 and UA1 causes peak value increases of temperatures at P1, P2 and P3 of 3°C (44.0°C to 47°C), 15°C (from 76°C to 91°C) and 6°C (from 59°C to 65°C). The maximum values of thermal conductivity of Layers USC, UT, UA23 and UA1 causes peak value decreases of temperatures at P1, P2 and P3 of 2°C (44.0°C to 42°C), 12°C (from 76°C to 64.0°C) and 9°C (from 59°C to 50°C)



Figure 24: Temperatures at Point P1 (Px/2) from Base Case and Cases with Maximum or Minimum Values of Thermal Conductivity, Equivalent Density or Thermal Capacity



Figure 25: Temperatures at Point P2 (cell centre) from Base Case and Cases with Maximum or Minimum Values of Thermal Conductivity, Equivalent Density or Thermal Capacity



## Figure 26: Temperatures at Point P3 ( $2.5\phi_{cell}$ ) from Base Case and Cases with Maximum or Minimum Values of Thermal Conductivity, Equivalent Density or Thermal Capacity

Figure 27 shows the influence of the minimum permeability, the minimum thermal conductivity, the maximum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the pore pressures at P1. All of these parameter values increase the pore water pressures. The sequence of parameters of minimum values with greatest to least influence on pore water pressure at P1 is:

Permeability > Thermal conductivity > Porosity > Specific heat Capacity > Young's modulus > Poisson's ratio > equivalent density > Thermal expansion.

The minimum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of pore pressure to increase from 12.3 MPa to 15.7 MPa (an increase of 28%).



Figure 27: Pore Pressure at P1 (Px/2) for the Base Case and Cases which Cause the Pressure Increase

Figure 28 shows the influence of the maximum permeability, the maximum thermal conductivity, the minimum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density, maximum Biot coefficient and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the pore pressures at P1. All these parameter values decrease the pore water pressures. The sequence of parameters of maximum values with greatest to least influence on pore pressure at P1 is:

Permeability > Young's modulus > Thermal conductivity > Porosity > Biot coefficient > Specific heat Capacity > Poisson's ratio > equivalent density > Thermal expansion.

The maximum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of pore pressure to decrease from 12.3 MPa to 9.2 MPa (a decrease of 25%).



Figure 28: Pore Pressure at P1 (Px/2) for the Base Case and Cases which Cause the Pressure Decrease

Figure 29 shows the influence of the minimum permeability, the minimum thermal conductivity, the maximum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the pore pressures at P3. All these parameter values increase the pore water pressures. The sequence of parameters of minimum values with greatest to least influence on pore pressure at P3 is:

Permeability > Thermal conductivity > Porosity > Specific heat Capacity > Young's modulus > Poisson's ratio > equivalent density > Thermal expansion.

The minimum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of pore pressure to increase from 11.9 MPa at 40 years to 16.6 MPa at 6 year (an increase of 40%).



Figure 29: Pore Pressure at P3 (2.5 $\phi_{cell}$ ) for the Base Case and Cases which Cause the Pressure Increase

Figure 30 shows the influence of the maximum permeability, the maximum thermal conductivity, the minimum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density, maximum Biot coefficient and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the pore pressures at P3. All these parameter values decrease the pore water pressures. The sequence of parameters of maximum values with greatest to least influence on pore pressure at P3 is:

Permeability > Young's modulus > Thermal conductivity > Porosity > Biot coefficient > Specific heat Capacity > Poisson's ratio > equivalent density > Thermal expansion.

The maximum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of pore pressure to decrease from 11.9 MPa at 40 years to 9.1 MPa at 30 years (a decrease of 24%).



Figure 30: Pore Pressure at P3 (2.5 $\phi_{cell}$ ) for the Base Case and Cases which Cause the Pressure Decrease

Figure 31 shows the influence of the maximum permeability, the minimum thermal conductivity, the minimum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the X-directional stress at P1. All these parameter values increase the X-directional stresses at P1. The sequence of parameters of maximum values with greatest to least influence on stresses in the X-direction at P1 is:

Young's modulus > Thermal expansion> Poisson's ratio > Thermal conductivity > Permeability > Specific heat Capacity > Porosity > equivalent density.

The maximum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of the Xdirectional stress to increase from 18.2 MPa at 680 years to 20.6 MPa at 600 year (an increase of 13%).



Figure 31: Stresses in X-direction at P1 for the Base Case and Cases which Cause the Stress Increase

Figure 32 shows the influence of the minimum permeability, the maximum thermal conductivity, the maximum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density, maximum Biot coefficient and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the X-directional stress at P1. All these parameter values decrease the X-directional stresses at P1. The sequence of parameters of minimum values with greatest to least influence on stresses in the X-direction at P1 is:

Young's modulus > Thermal expansion> Permeability > Poisson's ratio > Thermal conductivity > Specific heat Capacity > Porosity > Biot coefficient > equivalent density.

The minimum Young's modulus of Layers USC, UT, UA23 and UA1 causes the peak value of the X-directional stress to decrease from 18.2 MPa at 680 years to 16.1 MPa at 1000 year (a decrease of 12%).



Figure 32: Stresses in X-direction at P1 for the Base Case and Cases which Cause the Stress Decrease

Figure 33 shows the influence of the maximum permeability, the minimum thermal conductivity, the minimum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the X-directional stress at P3. All these parameter values increase the X-directional stresses at P3. The sequence of parameters of maximum values with greatest to least influence on stresses in the X-direction at P3 is:

Young's modulus > Thermal expansion> Thermal conductivity > Permeability > Poisson's ratio > Porosity > Specific heat Capacity > equivalent density.

The maximum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of the Xdirectional stress to increase from 17.9 MPa to 21.1 MPa at 35 year (an increase of 18%).



Figure 33: Stresses in X-direction at P3 for the Base Case and Cases which Cause the Stress Increase

Figure 34 shows the influence of the minimum permeability, the maximum thermal conductivity, the maximum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density, maximum Biot coefficient and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the X-directional stress at P3. All these parameter values decrease the X-directional stresses at P3. The sequence of parameters of minimum values with greatest to least influence on stresses in the X-direction at P3 is:

Young's modulus > Thermal expansion> Permeability > Thermal conductivity > Porosity > Poisson's ratio > Biot coefficient > Specific heat Capacity > equivalent density.

The minimum Young's modulus of Layers USC, UT, UA23 and UA1 causes the peak value of the X-directional stress to decrease from 17.9 MPa at 35 years to 15.6 MPa at 1000 year (a decrease of 13%).



Figure 34: Stresses in X-direction at P3 for the Base Case and Cases which Cause the Stress Decrease

Figure 35 shows the influence of the maximum permeability, the minimum thermal conductivity, the minimum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Y-directional stress at P1. All these parameter values increase the Y-directional stresses at P1. The sequence of parameters of maximum values with greatest to least influence on stresses in the Y-direction at P1 is:

Young's modulus > Thermal expansion> Poisson's ratio > Permeability >Thermal conductivity > Specific heat Capacity > Porosity > equivalent density.

The maximum Young's modulus of Layers USC, UT, UA23 and UA1 causes the peak value of the Y-directional stress to increase from 21.9 MPa at 820 years to 24.0 MPa at 800 year (an increase of 10%).



Figure 35: Stresses in Y-direction at P1 for the Base Case and Cases which Cause the Stress Increase

Figure 36 shows the influence of the minimum permeability, the maximum thermal conductivity, the maximum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density, maximum Biot coefficient and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Y-directional stress at P1. All these parameter values decrease the X-directional stresses at P1. The sequence of parameters of minimum values with greatest to least influence on stresses in the Y-direction at P1 is:

Young's modulus > Thermal expansion> Permeability > Poisson's ratio > Thermal conductivity > Specific heat Capacity > Porosity > Biot coefficient > equivalent density.

The minimum Young's modulus of Layers USC, UT, UA23 and UA1 causes the peak value of the X-directional stress to decrease from 21.9 MPa at 820 years to 19.9 MPa at 1000 year (a decrease of 9%).



Figure 36: Stresses in Y-direction at P1 for the Base Case and Cases which Cause the Stress Decrease

Figure 37 shows the influence of the maximum permeability, the minimum thermal conductivity, the minimum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Y-directional stress at P3. All these parameter values increase the Y-directional stresses at P3. The sequence of parameters of maximum values with greatest to least influence on stresses in the Y-direction at P3 is:

Young's modulus > Thermal expansion> Thermal conductivity > Permeability > Poisson's ratio > Porosity > Specific heat Capacity > equivalent density.

The maximum Young's modulus of Layers USC, UT, UA23 and UA1 causes the peak value of the X-directional stress to increase from 24.2 MPa to 28.4 MPa at 15 year (an increase of 17%).



Figure 37: Stresses in Y-direction at P3 for the Base Case and Cases which Cause the Stress Increase

Figure 38 shows the influence of the minimum permeability, the maximum thermal conductivity, the maximum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density, maximum Biot coefficient and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Y-directional stress at P3. All these parameter values decrease the Y-directional stresses at P3. The sequence of parameters of minimum values with greatest to least influence on stresses in the X-direction at P3 is:

Young's modulus > Thermal expansion> Thermal conductivity > Permeability > Biot coefficient > Poisson's ratio > Porosity > Specific heat Capacity > equivalent density.

The minimum Young's modulus of Layers USC, UT, UA23 and UA1 causes the peak value of the X-directional stress to decrease from 24.2 MPa at 15 years to 20.7 MPa at 15 year (a decrease of 14%).



Figure 38: Stresses in Y-direction at P3 for the Base Case and Cases which Cause the Stress Decrease

Figure 39 shows the influence of the minimum permeability, the minimum thermal conductivity, the maximum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, maximum Biot coefficient and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Z-directional stress at P1. All these parameter values decrease the Z-directional stresses at P1. The sequence of parameters of minimum values with greatest to least influence on stresses in the Z-direction at P1 is:

Permeability > Biot coefficient > Thermal conductivity > Young's modulus > Porosity > Specific heat capacity > Poisson's ratio > Thermal expansion> equivalent density.

The minimum permeability of Layers USC, UT, UA23 and UA1 causes the lowest value of the Zdirectional stress to decrease from 9.9 MPa at 32 years to 8 MPa at 65 year (about a decrease of 19%).



Figure 39: Stresses in Z-direction at P1 for the Base Case and Cases which Cause the Stress Decrease

Figure 40 shows the influence of the maximum permeability, the maximum thermal conductivity, the minimum porosity, minimum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, maximum equivalent density and minimum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Z-directional stress at P1. All these parameter values increase the lowest value of the Z-directional stresses at P1. The sequence of parameters of maximum values with greatest to least influence on stresses in the Z-direction at P1 is:

Permeability > Young's modulus > Thermal conductivity > Porosity > Specific heat capacity > Poisson's ratio > Thermal expansion> equivalent density.

The maximum permeability of Layers USC, UT, UA23 and UA1 causes the lowest value of the Z-directional stress to increase from 9.9 MPa at 32 years to 11.4 MPa at 20 year (an increase of 15%).



Figure 40: Stresses in Z-direction at P1 for the Base Case and Cases which Cause the Stress Increase

Figure 41 shows the influence of the minimum permeability, the minimum thermal conductivity, the maximum porosity, maximum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, maximum Biot coefficient, minimum Young's modulus and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the Z-directional stress at P3. All these parameter values decrease the Z-directional stresses at P1. The sequence of parameters of minimum values with greatest to least influence on stresses in the Z-direction at P3 is:

Permeability > Biot coefficient > Thermal conductivity > Young's modulus > Porosity > Specific heat capacity > Poisson's ratio > Thermal expansion> equivalent density>Young's modulus.

The minimum permeability of Layers USC, UT, UA23 and UA1 causes the lowest value of the Zdirectional stress to decrease from 12.2 MPa at 85 years to 10.2 MPa at 240 year (about a decrease of 16%).



Figure 41: Stresses in Z-direction at P3 for the Base Case and Cases which Cause the Stress Decrease

Figure 42 shows the influence of the maximum permeability, the maximum thermal conductivity, the minimum porosity, maximum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, and maximum equivalent density of rock of Layers USC, UT, UA23 and UA1 on the Z-directional stress at P3. All these parameter values increase the lowest value of the Z-directional stresses at P3. The sequence of parameters of maximum values with greatest to least influence on stresses in the Z-direction at P3 is:

Permeability > Porosity > Specific heat capacity > Young's modulus > Thermal conductivity > equivalent density > Poisson's ratio.

The maximum permeability of Layers USC, UT, UA23 and UA1 causes the lowest value of the Z-directional stress to increase from 12.2 MPa at 85 years to 13.9 MPa at 65 year (an increase of 14%).



Figure 42: Stresses in Z-direction at P3 for the Base Case and Cases which Cause the Stress Increase

Figure 43 shows the influence of the minimum permeability, the minimum thermal conductivity, the maximum porosity, minimum Young's modulus, minimum specific heat capacity, maximum Poisson's ratio, minimum equivalent density, maximum Biot coefficient, minimum Young's modulus and maximum thermal expansion of rock of Layers USC, UT, UA23 and UA1 on the uplift at P4. All these parameter values increase the uplift at P4. The sequence of parameters of minimum values with greatest to least influence on uplift at P4 is:

Permeability > Thermal expansion> Young's modulus > Poisson's ratio > Biot coefficient > Specific heat capacity > Thermal conductivity > Porosity > equivalent density.

The minimum permeability of Layers USC, UT, UA23 and UA1 causes the peak value of the uplift to increase from 9.6 cm at 1570 years to 12.9 at 780 year (an increase of 34%).



Figure 43: Uplift at Point P4 for the Base Case and Cases which Cause Uplift Increase

Figure 44 shows the influence of the maximum permeability, the maximum thermal conductivity, maximum Young's modulus, maximum specific heat capacity, minimum Poisson's ratio, and maximum equivalent density of rock of Layers USC, UT, UA23 and UA1 on the uplift at P4. All these parameter values decrease the lowest value of the uplift at P4. The sequence of parameters of maximum values with greatest to least influence on uplift at P4 is:

Thermal expansion > Poisson's ratio > Permeability > Specific heat capacity > Thermal conductivity > equivalent density > Young's modulus.

The minimum thermal expansion of Layers USC, UT, UA23 and UA1 causes the lowest value of the Z-directional stress to decrease from 9.6 cm at 1570 years to 7.4 cm at 1700 year (a decrease of 23%).



Figure 44: Uplift at Point P4 for the Base Case and Cases which Cause Uplift Decrease

In summary, the three most important factors influencing temperatures are thermal conductivity, specific heat capacity and equivalent density with the most important factor being thermal conductivity. Assuming a minimum value for thermal conductivity results in a maximum temperature difference of 15°C.

The major significant six factors influencing the pore pressure are permeability, thermal conductivity, porosity, specific heat capacity, Young's modulus, and Biot coefficient with the most important factor being permeability. Assuming a minimum value for permeability results in a maximum pore pressure difference at P3 by 40%.

The major significant six factors influencing the ground surface uplift are permeability, thermal expansion, Young's modulus and Poisson's ratio with the most important factor being permeability. Assuming a minimum value for permeability results in a maximum uplift difference by 34%.

#### 6.2.2 Sensitivity Analyses of Parameters of Single Layer Rock

6.2.2.1 Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC Used on the THM Response

Figures 45 and 46 show the influence of the maximum permeability values of Layer UT, or UA1, or UA23 or USC used in the COMSOL model on the pore water pressure at Point P1 and Point P3, respectively. Though there are some influences of the maximum permeability values of Layer UT, or UA1, or USC used on the pore water pressure at later time (after 100 years), there is no influence on the pore pressure peak value. However, the influence of the maximum permeability value of Layer UA23 is significant and it can cause 24% underestimation of the peak pore pressure at Point P1 and 22% underestimation of the peak pore pressure at Point P3.



Figure 45: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Pore Pressure at Point P1



Figure 46: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Pore Pressure at Point P3

Figures 47, 48, 49, 50, 51 and 52 show the influence of the maximum permeability values of Layer UT, or UA1, or UA23 or USC used in the COMSOL model on the X-, Y-, Z-directional stresses at Points P1 and P3, respectively.

All of them show that there is no significant influence of the maximum permeability values of Layer UT, or UA1 or USC used in the modelling, but the influence of the maximum permeability value of Layer UA23 is significant and it can cause 15% overestimation of the horizontal stresses and 42% underestimation of the thermally-induced vertical stress change.



Figure 47: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on X-directional Stress at Point P1



Figure 48: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Y-directional Stress at Point P1



Figure 49: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Z-directional Stress at Point P1



Figure 50: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on X-directional Stress at Point P3



Figure 51: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Y-directional Stress at Point P3



Figure 52: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Z-directional Stress at Point P3

Figure 53 shows the influence of the maximum permeability values of Layer UT, or UA1, or UA23 or USC used in the COMSOL model on the uplift at Point P4. The results indicate that using the maximum permeability values of Layer UT, or UA1, or USC does not have significant difference in the peak value of the uplift at Point 4. However, the maximum permeability value of Layer UA23 does have a significant influence on the uplift at Point P4.



Figure 53: Influence of Maximum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Uplift at Point P4

6.2.2.2 Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC Used on the THM Response

Figures 54 and 55 show the influence of the minimum permeability values of Layer UT, or UA1, or UA23 or USC used in the COMSOL model on the pore water pressure at Point P1 and Point P3, respectively. Although there are some influences of the minimum permeability values of Layer UT, or UA1, or USC used on the pore water pressure at later time (after 100 years), there is no influence on the pore pressure peak value. However, the influence of the minimum permeability value of Layer UA23 is significant and it can cause 27% overestimation of the peak pore pressure at Point P1 and 36% overestimation of the peak pore pressure at Point P3.



Figure 54: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Pore Pressure at Point P1



Figure 55: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Pore Pressure at Point P3

Figures 56, 57, 58, 59, 60 and 61 show the influence of the minimum permeability values of Layer UT, or UA1, or UA23 or USC used in the COMSOL model on the X-, Y-, Z-directional stresses at Points P1 and P3, respectively.

All of them show that there is no significant influence of the minimum permeability values of Layer UT, UA1 or USC used in the modelling, but the influence of the minimum permeability value of Layer UA23 is significant.



Figure 56: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on X-directional Stress at Point P1



Figure 57: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on X-directional Stress at Point P3



Figure 58: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Y-directional Stress at Point P1



Figure 59: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Y-directional Stress at Point P3



Figure 60: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Z-directional Stress at Point P1



Figure 61: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC used on Z-directional Stress at Point P3

Figure 62 shows the influence of the minimum permeability values of Layer UT, or UA1, or UA23 or USC used in the COMSOL model on the uplift at Point P4. Using the minimum permeability values of Layer UT, or UA1, or USC does not have significant difference in the peak value of the uplift at Point 4. However, assuming the minimum permeability value of Layer UA23 has a significant influence on the uplift at Point P4.



Figure 62: Influence of Minimum Permeability Values of Layer UT, or UA1, or UA23 or USC on the Uplift at Point P4

6.2.2.3 Analysis of Maximum Thermal Conductivity Values of Layer USC or UT Used on the THM Response

Figure 63 shows the influence of the maximum thermal conductivity values of Layer UT or USC used in the COMSOL model on the temperature at Point P1, Point P2 and Point P3. The

influences of the maximum thermal conductivity values of Layer UT or USC used on the temperature at different locations are very minor because these layers are far from the repository.



Figure 63: Influence of Maximum Thermal Conductivity Values of Layer USC or UT used on Temperatures at Points P1, P2 and P3

Figure 64 shows the influence of the maximum thermal conductivity values of Layer UT or USC used in the COMSOL model on the pore pressure at Point P1 and Point P3. The influences of the maximum thermal conductivity values of Layer UT or USC used on the pore pressure at different locations are very minor.



Figure 64: Influence of Maximum Thermal Conductivity Values of Layer USC or UT on Pore Pressures at Points P1 and P3

Figure 65 shows the influence of the maximum thermal conductivity values of Layer UT or USC used in the COMSOL model on the uplift at Point P4. The influence of the maximum thermal conductivity values of Layer UT or USC used on the uplift at P4 are also very minor.



Figure 65: Influence of Maximum Thermal Conductivity Values of Layer USC or UT on the Uplift at Point P4

6.2.2.4 Influence of Minimum Thermal Conductivity Values of Layer USC or UT Used on the THM Response

Figure 66 shows the influence of the minimum thermal conductivity values of Layer UT or USC used in the COMSOL model on the temperature at Point P1, Point P2 and Point P3. The influences of the minimum thermal conductivity values of Layer UT or USC used on the temperature at different locations are very minor.



Figure 66: Influence of Minimum Thermal Conductivity Values of Layer USC or UT on Temperatures at Points P1, P2 and P3

Figure 67 shows the influence of the minimum thermal conductivity values of Layer UT or USC used in the COMSOL model on the pore pressure at Point P1 and Point P3. The influences of the minimum thermal conductivity values of Layer UT or USC used on the pore pressure at different locations are very minor.



Figure 67: Influence of Minimum Thermal Conductivity Values of Layer USC or UT used on Pore Pressures at Points P1 and P3

Figure 68 shows the influence of the minimum thermal conductivity values of Layer UT or USC used in the COMSOL model on the uplift at Point P4. The influence of the minimum thermal conductivity values of Layer UT or USC used on the uplift at P4 are very minor.



Figure 68: Influence of Minimum Thermal Conductivity Values of Layer USC or UT used on the Uplift at Point P4

6.2.2.5 Influence of Maximum Young's Modulus Values of Layer UA23, or UT, or UA1, or USC Used in the COMSOL Model

Figure 69 show the influence of the maximum Young's modulus of Layer UA23, or UA1, or UT, or USC used in the COMSOL model on the pore pressure at Point P1 and Point P3, respectively. There is no influence of using maximum Young's modulus values of Layer UA1, or UT, or USC instead of using the mean values on the pore water pressure. But using the maximum value of the Young's modulus of Layer 23 can overestimate 7% of the peak value of the pore pressure.



Figure 69: Influence of Maximum/Minimum Young's Modulus Values of Layer UA23, or UT, or UA1, or USC used in the COMSOL Model on Pore Pressures at Points P1 and P3

Figure 70 shows the influence of the maximum Young's modulus of Layer UA23, or UA1, or UT, or USC used in the COMSOL model on the uplift at Point P3. The influence of using the maximum value of Young's modulus of Layer UA1, or UT or USC only has very minor influence on the uplift at Point P3. But using maximum Young's modulus value of Layer UA23 instead of mean value underestimates the uplift on P3 by 15% at Year 10 and overestimates by 3% at Year 5,000.



Figure 70: Influence of Maximum Young's Modulus Values of Layer UA23, or UT, or UA1, or USC used on the Uplift at Point P4

In summary, the major factors influencing the THM responses of the deep geological repository are the THM parameters of Layer UA23 which hosts the deep geological repository. The THM parameters in the layers above or below Layer UA23 does have an influence on the THM responses but differences are very minor.

#### 6.3 SENSITIVITY ANALYSES OF THE BOUNDARY CONDITIONS USING 3D MODEL

## 6.3.1 Sensitivity Analysis of the Hydraulic Boundary Condition Applied at the Bottom of the Model

Figure 71 shows the influence of using fixed pore pressure boundary condition on the model bottom surface instead of no-flow boundary condition used in the Base Case on the pore pressure at Point P1 and P3. It shows that there is no influence and this indicates that the vertical dimension is large enough to perform the model.



Figure 71: Influence of Hydraulic Boundary Condition on the Bottom of the Model on the Pore pressure at P1 and P3

Figure 72 shows the influence of using fixed pore pressure boundary condition on the model bottom surface instead of no-flow boundary condition used in the Base Case on the uplift at Point P4 (ground surface). There is no influence and this also indicates that the vertical dimension sufficient and boundary conditions are not driving model results.



Figure 72: Influence of Hydraulic Boundary Condition on the Bottom of the Model on the Uplift at P4

# 6.3.2 Sensitivity Analysis of the Thermal Boundary Condition on the Outside Vertical Surface

Figure 73 shows the influence of using no heat flow boundary condition used on the front and right side vertical surfaces of the model instead of using fixed temperature boundary condition used in the Base Case on the temperature at Points P1, P2 and P3. No differences were observed suggesting model boundary conditions are not driving model results.



Figure 73: Influence of Hydraulic Boundary Condition on the Front and Right Side Surfaces of the Model on the Temperature at Points P1, P2 and P3

Figure 74 shows the influence of using no heat flow boundary condition used on the front and right side vertical surfaces of the model instead of using fixed temperature boundary condition used in the Base Case on the pore pressure at Points P1 and P3. No differences were observed suggesting model boundary conditions are not driving model results.



Figure 74: Influence of Hydraulic Boundary Condition on the Front and Right Side Surfaces of the Model on the Pore Pressure at Points P1 and P3

#### 6.3.3 Sensitivity Analysis of the Galley Wall Boundary Conditions

Figure 75 shows the influence of assuming the buffer materials fully saturated at start instead of using atmospheric boundary condition on the gallery wall on the pore water pressure at Point P1 and Point P3. During the first 60 years, there is no influence. After 60 years, assuming the galleries are filled with fully saturated buffer materials greatly overestimates pore pressures at both Points P1 and P3.



Figure 75: Influence of Access/Connection Tunnels filled with Fully-saturated Buffer after 2 Years on the Pore Pressure at Points P1 and P3

Figure 76 shows the influence of assuming the buffer materials fully are saturated after 1000 years instead of using atmospheric boundary condition on the gallery wall on the pore water pressure at Point P1 and Point P3. During the first 1000 years, there is no influence. After 1000 years, assuming the galleries are filled with buffer materials fully saturated after 1000 years overestimates pore pressures at both Points P1 and P3.



Figure 76: Influence of Access/Connection Tunnels filled with Buffer after 1000 Years on the Pore Pressure at Points P1 and P3

Figures 77 and 78 show the influence of assuming the buffer materials are fully saturated at start instead of using atmospheric boundary condition on the gallery wall on the X-, Y- and Z-directional stresses at Point P1 and Point P3, respectively. At both locations, there is no influence for the first 60 years. After 60 years, assuming the buffer materials are fully saturated at start instead of using atmospheric boundary condition slightly decreases the X- and Y-directional stresses. However, it significantly decreases the Z-directional stress.



Figure 77: Influence of Access/Connection Tunnels filled with Buffer after 2 Years on Stresses at Point P1



Figure 78: Influence of Access/Connection Tunnels filled with Buffer after 2 Years on Stresses at Point P3
Figures 79 and 80 show the influence of assuming the buffer materials fully saturated after 1000 years instead of using atmospheric boundary condition on the gallery wall on the X-, Y- and Z-directional stresses at Point P1 and Point P3, respectively. At both locations, there is no significant influence on the X- and Y-directional stresses. For the Z-directional stress, there is only slightly influence after 1000 years.



Figure 79: Influence of Access/Connection Tunnels filled with Buffer after 1000 Years on Stresses at Point P1



Figure 80: Influence of Access/Connection Tunnels filled with Buffer after 1000 Years on Stresses at Point P3

Figure 81 shows the influence of assuming the buffer materials in galleries are fully saturated after two years or after 1000 years on the uplift at Point P4. Assuming the galleries are filled

with fully saturate buffer material after two years overestimate the peak uplift by 14%. Assuming the galleries are filled with buffer materials fully saturated after 1000 years overestimated peak value by 6%.



Figure 81: Influence of Access/Connection Tunnels filled with Buffer after 2 years or 1000 Years on Stresses at Point P4

# 6.3.4 Sensitivity Analysis of the HA Cell Boundary Conditions

Figure 82 shows the influence of using fixed boundary condition on the cell wall (representing the steel line) instead of free boundary condition used in the Base Case on the pore pressure at Points P1 and P3. There is no noticeable influence.



Figure 82: Influence of Fixed Boundary Condition on the Cell Wall after 2 Years on the Pore Pressure at Points P1 and P3

Figures 83, 84 and 85 show the influence of using fixed boundary condition on the cell wall instead of free boundary condition used in the Base Case on the X-, Y- and Z-dimensional stresses, respectively. Fixed boundary condition on the cell wall instead of the free boundary conditions increases the peak X-directional stress at Point P3 about 1.3 MPa and decreases the Z-directional stress at P3 less than 0.5 MPa. It does not have any influence on the Y-directional stress at Point P3. It also does not influence the stresses at Point P1.



Figure 83: Influence of Fixed Boundary Condition on the Cell Wall after 2 Years on the Xdirectional Stress at Points P1 and P3



Figure 84: Influence of Fixed Boundary Condition on the Cell Wall after 2 Years on the Ydirectional Stress at Points P1 and P3



# Figure 85: Influence of Fixed Boundary Condition on the Cell Wall after 2 Years on the Zdirectional Stress at Points P1 and P3

In summary, model results are not sensitive to exterior model hydraulic or thermal model boundary conditions. This indicates the model domain (2 km x 2.5 km x 3 km) is appropriate and results are not influenced by boundary conditions.

The boundary conditions on the gallery wall has influence on the pore water pressure but does not influence the peak value. Assuming the galleries filled with fully saturated buffer materials after 2 years overestimates the ground surface uplift by 14%.

Using fixed boundary condition on the cell wall does not influence the pore pressure. Horizontal stress near the cell were affected but stresses at the mid-point between two cells was not. There was a small influence of the fixed boundary condition on the vertical stress near the cell wall.

# 6.4 SENSITIVITY ANALYSIS OF THE NUMBER OF INDIVIDUAL PLACEMENT CELLS IN DETAIL PRESENTED IN THE COMSOL MODEL USING 3D MODEL

Figure 86 shows the comparison of temperature at P1, P2 and P3 between the models in which there are 2, 4, 6 and 8 individual placement cells in detail presented. There is no noticeable difference in temperatures at these locations.



Figure 86: Influence of the Number of Individual Placement Cells in Detail Presented on Temperatures at Points P1, P2 and P3

Figure 87 shows the comparison of pore pressure at P1 and P3 between the models in which there are 2, 4, 6 and 8 individual placement cells in detail presented. The pore pressure at both P1 and P3 are slightly lower when there are only 2 or 4 individual cells in detail presented than that when 6 or 8 individual cells in detail are presented. There is no noticeable difference in pore pressure between the models including 6 or 8 individual cells in detail presented and this indicates that for this model six individual cells in detail presented are good enough to perform this simulation.



Figure 87: Influence of the Number of individual Cells in Detail Presented on Pore Pressures at Points P1, P2 and P3

Figures 88, 89 and 90 show the comparison of the X-, Y-, and Z-directional stresses at P1 and P3 between the models in which there are 2, 4, 6 and 8 individual cells in detail presented. There are slight difference between the models including only 2 or 4 individual cells in detail presented and the models including 6 or 8 individual cells in detail presented. There is no noticeable difference in stresses between the models including 6 or 8 individual cells in detail presented and this also indicates that for this model six cells with details are good enough to perform this simulation.



Figure 88: Influence of the Number of Individual Cells in Detail Presented on the Xdirectional Stress at Points P1 and P3



Figure 89: Influence of the Number of Individual Cells in Detail Presented on the Ydirectional Stress at Points P1 and P3



Figure 90: Influence of the Number of Individual Cells in Detail Presented on the Zdirectional Stress at Points P1 and P3

In summary, simplification of using the block to represent the cells does not have any influence on the THM results at locations near a panel centre as long as there are 6 or more individual cells in detail presented near the panel centre are incorporated in the model.

## 6.5 INFLUENCE OF VERTICAL DIMENSIONS ON THE THM RESULTS USING 3D MODEL

Figure 91 compares the temperatures at P1, P2 and P3 when the model vertical dimensions are 1135 m, 1635 m, and 2635 m with temperature from Base Case model which has vertical dimension of 3000 m. There is no difference in temperature at any point. This means from the point of view of thermal component the vertical model dimension is not driving the model results and a smaller domain could be used.



Figure 91: Influence of Vertical Model Size on Temperatures at Points P1, P2 and P3

Figure 92 compares the pore pressures at P1 and P3 when the model vertical dimensions are 1135 m, 1635 m, and 2635 m with pore pressures from Base Case model which has vertical dimension of 3000 m. There is no difference in pore pressure at any point. This means from the point of view of hydraulic component the vertical model dimension is not driving the model results and a smaller domain could be used.



Figure 92: Influence of Vertical Model Size on Pore Pressure at Points P1 and P3

Figure 93 compares the uplift at P4 when the model vertical dimensions are 1135 m, 1635 m, and 2635 m with the uplift from Base Case model which has vertical dimension of 3000 m. There is no obvious difference in the uplift at P4 (ground surface) between models with vertical dimensions of 2635 m and Base but with smaller dimensions (e.g., 1135 m or 1635 m) the uplift was underestimated. This means the uplift is sensitive to the vertical model dimension but a somewhat smaller model domain could be used (i.e., 2635 m or more).



Figure 93: Influence of Vertical Model Size on Uplift at Point P4

## 6.6 INFLUENCE OF USING 4 PANELS INSTEAD OF 6 PANELS USING 3D MODEL

Figure 94 compares the temperatures at P1, P2 and P3 from the model including 4 panels with those from Base Case which includes 6 panels. There is no noticeable differences at these three points.



Figure 94: Influence of using Four Panels to represent Six Panels on Temperatures at Points P1, P2 and P3

Figure 95 compares the pore pressures at P1 and P3 from the model including 4 panels with those from Base Case which includes 6 panels. There is no noticeable differences at these two points.



Figure 95: Influence of using Four Panels to represent Six Panels on Pore Pressure at Points P1 and P3

Figures 96, 97 and 98 compare the X-, Y- and Z-directional stresses at P1 and P3 from the model including 4 panels with those from Base Case which includes 6 panels. There is no noticeable differences at these two points.



Figure 96: Influence of using Four Panels to represent Six Panels on the X-directional Stress at Points P1 and P3



Figure 97: Influence of using Four Panels to represent Six Panels on the Y-directional Stress at Points P1 and P3



Figure 98: Influence of using Four Panels to represent Six Panels on the Z-directional Stress at Points P1 and P3

Figure 99 compares the uplift at P4 from the model including 4 panels with those from Base Case which includes 6 panels. The uplift at P4 from the model including 4 panels is underestimated by 8%.



Figure 99: Influence of using Four Panels to represent Six Panels on Uplift at Point P4

In summary, using the model incorporating 4 panels to model the HLW repository in the case study based on Cigéo data (the Cigéo project has 24 panels and six panels should be used considering symmetry) does not have any influence on the THM response at the locations near the panel centre but it underestimates the ground surface uplift by 8%.

# 7. VALIDATION

There are no available direct theoretical solution or physical test results for this complicated model at this moment. To validate this model, two steps are taken. The first step is to validate the theoretical equations used for this model by comparing the THM response in an infinite rock mass with a point heat source with the theoretical solution provided by Smith and Booker (1993). The second step is to validate the coupled COMSOL THM model for the HLW repository in the case study by comparing the thermal components from the Base case calculation with the calculated results from Guo (2017), which can provide accurate thermal results for a deep geological repository.

# 7.1 VALIDATION OF THE THEORETICAL EQUATIONS

When a point heat source is buried in a saturated soil, the temperature changes that occur will cause the pore water to expand a greater amount than the voids of the soil. If the soil is sufficiently permeable these pore pressures will dissipate. Smith and Booker (1993) developed a general analytical solution for a linear theory of thermo-poroelastic consolidation in a homogeneous isotropic material.

In the validation model using the geometry shown in Figure 100, the initial temperature, pore water pressure and stresses are set to 0°C, 0 MPa, and 0 MPa. Thermal and hydraulic conditions use symmetry and the three symmetric planes (x = 0 m, y = 0 m, and z = 0 m) are defined as impermeable and adiabatic. At external model boundaries, the temperature and pore pressure are set to 0°C and 0 Pa. A constant point power of Q = 700 W /8 = 87.5 W is applied at point (0, 0, 0). Regarding mechanical conditions, all boundaries are free except the symmetric planes (x = 0 m, y = 0 m, and z = 0 m) where a roller boundary condition is applied.



Figure 100: COMSOL Point Heat Source Model Geometry

For the purpose of validation, the material in the packer borehole is assumed to be rock material for consistency with Smith and Booker (1993). The rock and water parameters used are as shown in Table 10.

| Parameters   | Rock                  | Water              |
|--|-----------------------|--------------------|
| Initial porosity                                       | 0.15                  | _                  |
| Equivalent thermal conductivity of rock (W/(m·K))      | 1.7                   | -                  |
| Equivalent density of rock (kg/m <sup>3</sup> )        | 2400                  | _                  |
| Equivalent heat capacity of rock (J/(kg·K))            | 1000                  | _                  |
| Permeability (m <sup>2</sup> )                         | 4.5x10 <sup>-20</sup> | _                  |
| Young's modulus (MPa)                                  | 4500                  | _                  |
| Poisson's ratio  | 0.3                   | _                  |
| Rock volumetric thermal expansion<br>coefficient (1/K) | 4.2x10 <sup>-5</sup>  | -                  |
| Reference density of water (kg/m <sup>3</sup> )        | _                     | 1000               |
| Compressibility of water (1/Pa)                        | _                     | 0                  |
| Heat capacity of water (J/(kg·K))                      | _                     | 4180               |
| Dynamic viscosity of water (Pa·s)                      | _                     | 1x10 <sup>-3</sup> |
| Water volumetric thermal expansion coefficient (1/K)   | -                     | 4x10 <sup>-4</sup> |
| Biot coefficient                                       | 0.6                   |                    |

|  | Table | 10: Material | Parameters | Used in the | COMSOL | . Point Heat | Source Mode | ł |
|--|-------|--------------|------------|-------------|--------|--------------|-------------|---|
|--|-------|--------------|------------|-------------|--------|--------------|-------------|---|

The modelled temperatures, pore water pressures, displacements and normal stresses at points P1 (0.35, 0, 0), P2 (0.5, 0, 0), P3 (1.5, 0, 0) and P4 (0.35, 0.5, 0.6) are compared with the theoretical solutions below.

Figure 101 shows the comparison of the temperatures calculated using the COMSOL model with theoretical solutions at points P1, P2, P3 and P4. The calculated temperatures match the theoretical solution exactly.



Figure 101: Comparison of Temperatures Calculated using the COMSOL Model and the Theoretical Solution at Points P1, P2, P3 and P4

Figure 102 shows the comparison of the pore water pressure calculated using the COMSOL model and the theoretical solution at points P1, P2, P3 and P4. The calculated pore water pressures match the theoretical solution exactly.



Figure 102: Comparison of Pore Pressures Calculated using the COMSOL Model and the Theoretical Solution at Points P1, P2, P3 and P4

Figure 103 shows the comparison of the displacements calculated using the COMSOL model and the theoretical solution at Point P4. The calculated displacement match the theoretical solution excellent.



Figure 103: Comparison of Displacements Calculated using the COMSOL Model and the Theoretical Solution at Point P4

# Figures 1043 shows the comparison of the normal stresses in three directions calculated using the COMSOL model and the theoretical solution at Point P4. The calculated stresses match the theoretical solution exactly.



Figure 104: Comparison of Normal Stresses Calculated using the COMSOL Model and the Theoretical Solution at Point P4

In summary, the excellent agreement between the numerical model and the analytical solutions indicates that the conceptual THM coupled model can be used to correctly model coupled THM processes in a fully saturated geotechnical material.

# 7.2 VALIDATION OF THE 3D COMSOL MODEL

In this study, only six detailed cells were incorporated to simplify the model and reduce the calculation time. The accuracy of this simplification needs to be validated. Guo (2017)

proposed a method which can calculate accurate temperatures at any location in a deep geological repository. To validate the coupled THM COMSOL model, the method proposed in Guo (2017) was used to calculate the thermal components. The calculated results using the method proposed in Guo (2017) are compared with the thermal results from the Base Case modelling.

Figures 105, 106 and 107 show the comparison of temperatures at Point P1, P2 and P3 from the coupled THM COMSOL model for the Base Case with the accurate results with an excellent agreement. This indicates the models in Section 4 are correctly built.



Figure 105: Comparison of Temperature between Coupled THM COMSOL Model and the Accurate Results at Point P1



Figure 106: Comparison of Temperature between Coupled THM COMSOL Model and the Accurate Results at Point P2



Figure 107: Comparison of Temperature between Coupled THM COMSOL Model and the Accurate Results at Point P3

# 8. CONCLUSIONS

A series of 2D or 3D coupled THM modelling has been performed to gain a better understanding of the thermal, hydraulic and mechanical response in the COx for the near field and far-field areas of the HLW repository case study. The theory used to perform the coupled THM modelling is validated by comparing the modelled THM results for a point heat source in an infinite rock mass with the theoretical solution by Smith and Booker (1993). The coupled COMSOL model for the HLW repository case study is also validated by comparing its thermal component for the Base Case with accurate results calculated using Guo (2017).

The modelling results from the Base Case model show:

- The cell centre temperature reaches its peak value of 75.8°C after 11.8 years of gallery excavation; The temperature at 2.5Φ<sub>cell</sub> reaches its peak of 59°C after 29.7 years; and the temperature at mid-point (Px/2)) between two cells reaches its peak 44°C after 387 years.
- The peak pore pressures are 12.0 MPa at point 2.5Φ<sub>cell</sub> after 40 years and 12.3 MPa at Point Px/2 after 38 years.
- The peak X-directional stresses are 17.9 MPa at point  $2.5\Phi_{cell}$  after 35 years and 18.2 MPa at Point Px/2 after 680 years.
- The peak Y-directional stresses are 24.2 MPa at point  $2.5\Phi_{cell}$  after 15 years and 21.9 MPa at Point Px/2 after 820 years.
- The lowest Z-directional stresses are 12.2 MPa at point  $2.5\Phi_{cell}$  after 85 years and 9.9 MPa at Point Px/2 after 32 years.
- The simulated uplift on the ground surface above the panel centre reaches its peak of 9.6 cm after 1570 years.

The thermal results from the 2D and 3D models were found to have the best agreement within the first 100 years, the hydraulic results had a good agreement within the first 40 years and the mechanical results also had a good agreement within 40 years. Maximum observed temperature difference was 3°C at different locations and occurred at 700 years, maximum observed pore pressure difference was 3.7 MPa at both Point  $2.5\Phi_{cell}$  and Point Px/2 and occurred at 500 years, maximum observed vertical stress differences were 1.6 MPa at Point Px/2 and 2.7 MPa at Point  $2.5\Phi_{cell}$ , and maximum observed ground surface uplift increase was 6.1 cm (an increase of 64%).

The most important factor influencing temperature is thermal conductivity. Assuming the minimum value of thermal conductivity of COx could cause temperature overestimates of 3°C at Point Px/2, 15°C at cell centre and 6°C at Point  $2.5\Phi_{cell}$  and assuming the maximum value of thermal conductivity of COx could underestimate temperature 2°C at Point Px/2, 12°C at cell centre and 9°C at Point  $2.5\Phi_{cell}$ .

The most important factor influencing pore pressure is rock permeability. Assuming the maximum value of permeability of COx could cause pore pressure increases of 28% at Point Px/2 and 40% at Point  $2.5\Phi_{cell}$  and assuming the minimum value of permeability of COx causes pore pressure decreases of 25% at Point Px/2 and 24% at Point  $2.5\Phi_{cell}$ .

The most important factors influencing the ground surface uplift are rock thermal expansion and rock permeability. Assuming the minimum permeability of COx could increase the ground surface uplift estimation by 34%, while assuming the minimum rock thermal expansion could decrease the ground surface uplift estimation by 23%.

The influence of the THM parameters of the rock above or below Layer UA23 on the THM response in near-field or far-field results are very minor.

As long as the dimension sizes are large enough, the bottom hydraulic boundary condition and the thermal/hydraulic boundary condition on the far-field outside vertical surfaces do not have any influence on the THM modelling results.

Assuming the buffer materials in the galleries is fully saturated after 1000 year only slightly influences pore pressure, stresses and ground surface uplift after 1000 years. Assuming the galleries are filled with fully saturated buffer materials can cause pore pressure increases only after 60 years but does not influence the peak value. Assuming the galleries are filled with fully saturated buffer materials can cause by 6%.

Applying the fixed mechanical boundary condition on the cell wall only slightly influences the horizontal stress which is perpendicular to the cell axis.

As long as there are six or more individual placement cells in detail presented in the COMSOL model, using blocks to represent the other placement cells to simplify the coupled THM model is good enough to perform the coupled THM modelling.

One quarter of the HLW repository in the case study based on Cigéo data includes six placement panels which are used in the Base Case. Although using the model incorporating four placement panels does not have any significant influence on the thermal, hydraulic and mechanical response in the near-field results (at Points P1, P2 and P3), it does influence the far-field results (decreasing 8% ground surface uplift at Point P4).

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