



# Thermal management associated with geologic disposal of large spent nuclear fuel canisters in tunnels with thermally engineered backfill

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## ARTICLE INFO

### Keywords:

Nuclear waste disposal  
Coupled processes modeling  
Thermal management  
Rock stress

## ABSTRACT

Coupled thermal-hydro-mechanical (THM) numerical modeling is conducted to study thermal management associated with geologic disposal of spent nuclear fuel (SNF) in large dual-purpose canisters (DPCs). DPCs, are containers designed for SNF storage and transportation and if determined to be feasible for permanent geological disposal could provide a cost effective disposal solution. However, one of the challenges to direct disposal of DPCs is thermal management to avoid overheating of the Engineered Barrier System (EBS), including bentonite-backfill used as a protective buffer. The model simulations show that the use of a backfill that is thermally engineered for high heat conduction can reduce the EBS temperature to acceptable levels for disposal of large waste canisters in backfilled tunnels. On the other hand, the use of high heat conduction backfill will not reduce the far field rock peak temperature that can occur several thousand years after closure of the repository. This longer term host rock peak temperature generates thermal-poro-elastic stress and geomechanical changes that must be considered in the thermal management and design of a repository.

## 1. Introduction

Deep geological disposal of high-level radioactive nuclear waste is investigated in many countries considering various host rocks (Faybishenko et al., 2016). The most widely proposed geological disposal concept is a mined repository in which waste encapsulated in metal canisters that are emplaced into excavations and then embedded in backfilled material, such as bentonite (Ahn and Apted, 2010). The design of the Engineered Barrier System (EBS) includes waste canister materials, as well as backfill material, which varies depending on the type of waste and the host rock. The EBS, including the backfill (or buffer) plays a significant role in the containment as well as for providing mechanical stability to the canisters and excavations during the post-closure temperature increase in the EBS and host rock (Rutqvist et al., 2005, 2014).

Currently, the U.S. Department of Energy (DOE) is investigating the feasibility of deep geological disposal of Spent Nuclear Fuel (SNF) in dual-purpose canisters (DPCs). DPCs are large containers used for storage and transportation, but not designed for long-term geologic disposal (Hardin et al., 2013, 2014, 2015). If DPCs are determined to be suitable for disposal, substantial cost savings could be made by eliminating the need for cutting the storage canisters open and repackaging the spent fuel into new disposal canisters. Each DPC would be sealed in a purpose-designed overpack for long-term disposal. The overpack

would be robust, and provide structural support for handling, transport, underground emplacement, and containment through the period of repository operations (Hardin et al., 2014).

DPCs containing 24 Pressurized Water Reactor (PWR) fuel elements are common and DPCs may contain up to 37 PWR elements in the future (Hardin et al., 2013). DPCs with up to 37 PWR elements are very large compared to more conventional disposal canisters, such as those used in the Swedish KBS-3 concept, containing just 4 PWR elements (Posiva, 2017; Cho et al., 2007). Since the amount of decay heat released from a specific waste canister depends on the number of spent fuel elements, very high temperatures could be expected around DPCs containing 24 or 37 PWR elements. As a result, post-closure thermal management strategies that allow for disposal within 150 years (after taken out of the reactor) have been identified as one of the challenging aspects of direct DPC disposal (Hardin et al., 2015). Thermal management strategies include keeping emplacement tunnels open with ventilation for decades, because backfill generally leads to a substantial increase in temperature at the waste package. Thus, it is not clear whether a multi-barrier repository design with bentonite-backfilled tunnels are feasible for disposal of large sized nuclear waste canisters.

Thermal management associated with geologic nuclear waste disposal, including studies related to direct DPC disposal, is usually based on managing the peak temperature at the waste canister and the bentonite buffer (Posiva, 2017; Leupin et al., 2016; Cho et al., 2007; Hardin

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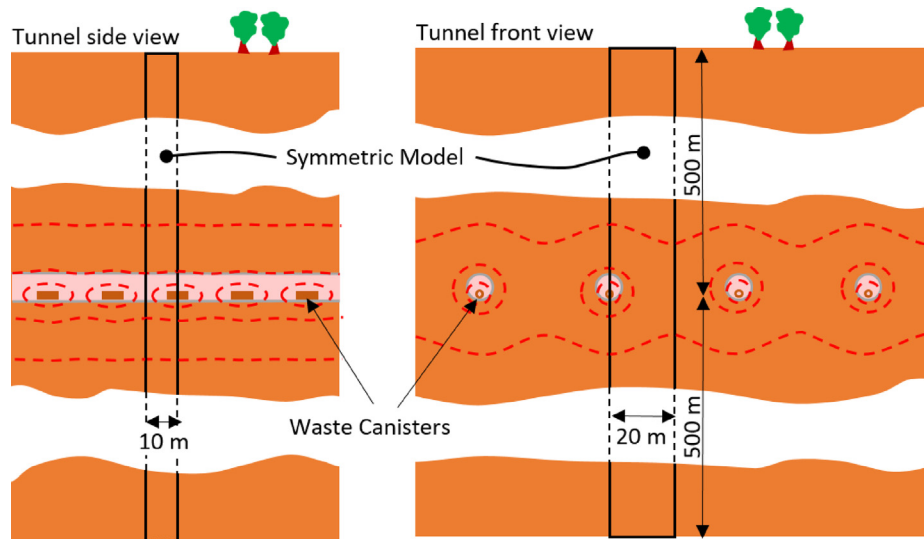
<https://doi.org/10.1016/j.tust.2020.103454>

Received 24 January 2020; Received in revised form 28 April 2020; Accepted 12 May 2020

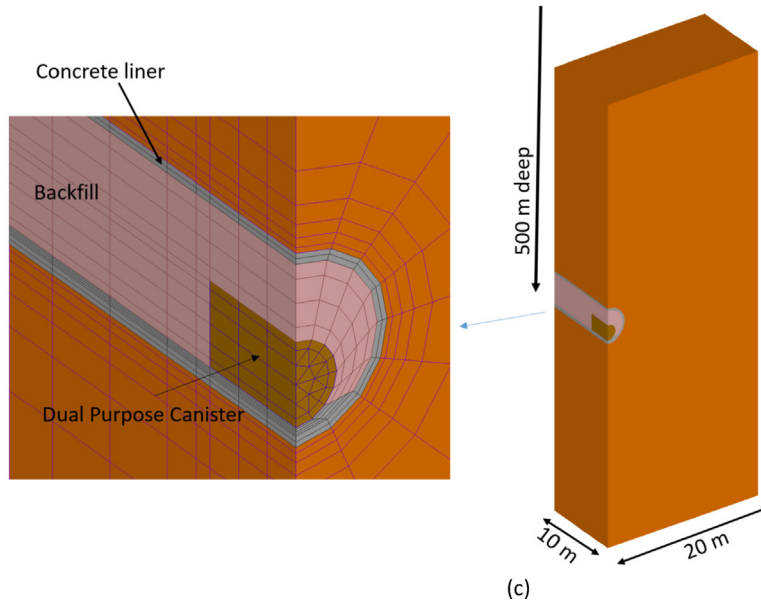
Available online 23 May 2020

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(a)



(b)

(c)

Fig. 1. Three-dimensional model geometry of a horizontal emplacement tunnel in the middle of a repository with 20 m center-to-center spacing between individual DPCs and 40 m spacing between individual emplacement tunnels. (a) Tunnel side and front views illustrating the symmetric temperature evolution with the numerical grid and 3D view shown in (b) and (c).

et al., 2013, 2015). For example, in the Swedish, Finnish and Korean nuclear waste programs, considering KBS-3 like waste disposal concepts in crystalline rock, it is required that the temperature at the canister surface should not exceed 100 °C, to assure chemical stability of the bentonite (Posiva, 2017). It is recognized that at higher temperatures, such as above 150 °C, mineral transformation can take place so that bentonite swelling capacity decreases and permeability increases (Sellin and Leupin, 2013). In the Swiss nuclear waste disposal concept, with bentonite backfilled tunnels in tight clay stone (Opalinus Clay), temperatures higher than 100 °C is tolerated for the bentonite, because the host rock is a primary barrier (Leupin et al., 2016). Instead, a temperature limit is set for the Opalinus Clay to be below the maximum paleotemperature of about 80 °C, thereby excluding thermally induced geochemical processes detrimental to host rock properties (Leupin et al., 2016). Recent modeling studies of long-term clay behavior around a heat source have indicated that temperatures as high as 200 °C may have some effect on the swelling stress by illitization (transfer of smectite to illite), although a reduction in swelling stress of only about

1 MPa was calculated (Zheng et al., 2015, 2017). One missing item here is the larger scale host rock temperature evolution that evolves over a longer term and will induce large scale coupled thermal-hydro-mechanical (THM) processes and geomechanical changes (Rutqvist et al., 2009a,b; 2014; Yoon and Zang, 2019). The relative importance of near-field and far-field temperature changes may depend on the size and decay heat of individual waste canisters, whether smaller sized 4 PWR canister or large sized 37 PWR canisters.

Related to EBS and nearfield host rock, a number of THM in situ heater experiments have been performed over the years and they have been complemented with laboratory experiments and interpretative coupled processes modeling (Birkholzer et al., 2019). Heater experiments in crystalline rocks include the Kamaishi Mine heater experiment in Japan (Rutqvist et al., 2001a), the FEBEX heater experiment at Grimsel Switzerland (Alonso, 2005), TSX heater test at the underground research laboratory in Manitoba, Canada (Gou and Dixon, 2006), and the Prototype Repository at Äspö Hard Rock Laboratory in Sweden (Thomas et al., 2013). In Situ heater experiments in argillaceous

claystone, or Argillite, include the HE-D and HE-E experiments at the Mont Terri Laboratory, Switzerland (Garitte et al., 2017a, 2017b), as well as the TED and ALC experiments at the Meuse/Haute-Marne underground research laboratory in France (Armand et al., 2017; Xu et al., 2020). These experiments have also been part of the international model comparison project DECOVALEX, which have significantly contributed to development of coupled processes numerical models and increased understanding of near field coupled THM processes in general (Birkholzer et al., 2019). Modeling of these types of in situ heater experiments have typically yielded that thermal processes can be predicted with confidence, while prediction of coupled hydraulic and mechanical processes are more uncertain as they are more complex and sensitive to local heterogeneities (e.g., Rutqvist et al., 2001a; Xu et al., 2020).

In this study, coupled THM processes modeling is applied to investigate key processes and parameters for thermal management associated with direct disposal of large sized DPCs in backfilled tunnels. Moreover, the use of thermally engineered backfill for reducing and controlling the relatively short term (tens of years) buffer peak temperature is investigated. Utilized are results from recently published laboratory experiments that have shown that the thermal conductivity of bentonite can be significantly increased by mixing in graphite or graphene oxide (Chen et al., 2018). The model simulations are performed using previously applied models with detailed representation of the near-field coupled THM processes in the EBS and rock system (Rutqvist et al., 2009a; 2011, 2014), but here for the first time applied to study direct disposal of large sized DPCs. The results presented are also relevant for other types of disposal canisters, including multi-purpose canisters that are canisters designed for all the steps of storage, transportation and disposal (Cumberland et al., 2015). Moreover, the results are generalized by studying two different host rock types: softer argillaceous clay (or argillite) and hard crystalline (granite) host rocks. The large sized and heavy DPCs implies that this study is focused on emplacement in horizontal tunnels, whereas other options of vertical emplacement exist, such in the aforementioned KBS-3 concept.

The next section (Section 2) presents the model setup, including model geometry, initial and boundary conditions, and material properties for both argillite and crystalline host rock options. This is followed in Section 3 by TH thermal management calculations to investigate the use of thermally engineered buffer properties that aims at managing the peak temperature in the EBS. In Section 4, key coupled THM processes in the host rock and their impact on thermal management are studied for disposal in argillite and crystalline host rocks. Section 5 provides a discussion on the key results with respect to thermal managements, followed by conclusions in Section 6.

## 2. Model setup

Figs. 1 and 2 present the model geometry for simulating disposal at 500 m depth in argillite and crystalline host rocks. As a result of repetitive symmetry, a three-dimensional symmetric model around one DPC is constructed to represent the evolution for an emplacement

tunnel at the inner part of a repository, where the highest temperature changes and thermal impact could be expected (Fig. 1). The 3D model is built for a canister-to-canister spacing of 20 m along the emplacement tunnels and 40 m spacing between individual emplacement tunnels (Fig. 1a). The DPCs with overpack (5.6 m long and 2 m in diameter) are placed on the floor of the emplacement tunnels of about 4.5 m in diameter (Hardin et al., 2013, 2014). The DPCs are assumed to have THM properties corresponding to steel, including Young's modulus  $E = 210$  GPa, Poisson's ratio  $\nu = 0.3$ , thermal conductivity  $\lambda = 20$  W/m $\cdot$ °C and specific heat  $C_s = 500$  J/kg $\cdot$ °C. In the case of an argillite host rock, the tunnels are reinforced with a concrete liner and the DPCs are placed on a concrete invert on the tunnel floor. In these simulations we consider that the EDZ is minor with same properties as the surrounding host rock.

As a result of the repetitive symmetry, the boundary conditions on the lateral boundaries of the 3D model are no heat or fluid flow and no displacements normal to the boundaries. On the top and bottom boundaries, temperature and fluid pressure is fixed, with vertical displacement fixed to zero on the bottom and free to move on the upper boundary representing the free moving ground surface. Further, the repetitive symmetry assumes that all neighboring DPCs are emplaced simultaneously to account for heat impact from neighboring DPCs.

Some of the basic THM properties for the host rocks and concrete liner are listed in Table 1. For the case of crystalline rock, properties are taken from previous modeling studies within the international DECOVALEX project (Rutqvist et al., 2009a,b), including properties derived from site investigations at the Äspö Hard Rock Laboratory in Sweden. For the case of argillite host rock, the rock properties correspond to those of Opalinus Clay at the Mont Terri Laboratory in Switzerland, a parameter set that has also been applied in previous coupled process models (Gens et al., 2007; Corkum and Martin, 2007; Rutqvist et al., 2014; Garitte et al., 2017a).

The backfill for the buffer is assumed to consist of the bentonite used in the Full-scale Engineered Barriers Experiment (FEBEX), at the Grimsel Test Site in Switzerland (Alonso, 2005; Gens et al., 2009). The bentonite THM model used here is the same as those used and presented in Rutqvist et al. (2011) with parameters listed in Table 2. In this study, the simpler linear swelling for the bentonite buffer was considered to provide a 5-MPa swelling stress upon full saturation (Rutqvist et al., 2011). The linear swelling model adds a swelling strain,  $\Delta\varepsilon_{sw}$ , according to  $\Delta\varepsilon_{sw} = \Delta S_l \times \beta_{sw}$ , where  $\Delta S_l$  is changes in liquid saturation and  $\beta_{sw}$  is a moisture swelling coefficient (Rutqvist et al., 2001b). For a bulk modulus of 20 MPa and  $\beta_{sw} = 0.238$ , a swelling stress of about 5 MPa is achieved after full saturation. The parameters for the water retention curve and relative permeability listed in Table 2 have in the past been determined through back-analysis modeling of laboratory experiments on FEBEX bentonite (Rutqvist and Tsang 2004; Alonso, 2005).

An important property for this study is the thermal conductivity of the buffer. Based on the FEBEX bentonite properties, in the numerical model, the thermal conductivity is linearly dependent on saturation varying from  $\lambda_{dry} = 0.5$  W/mK (at zero liquid saturation) to  $\lambda_{wet} = 1.3$  W/mK (at full liquid saturation). For the simulations

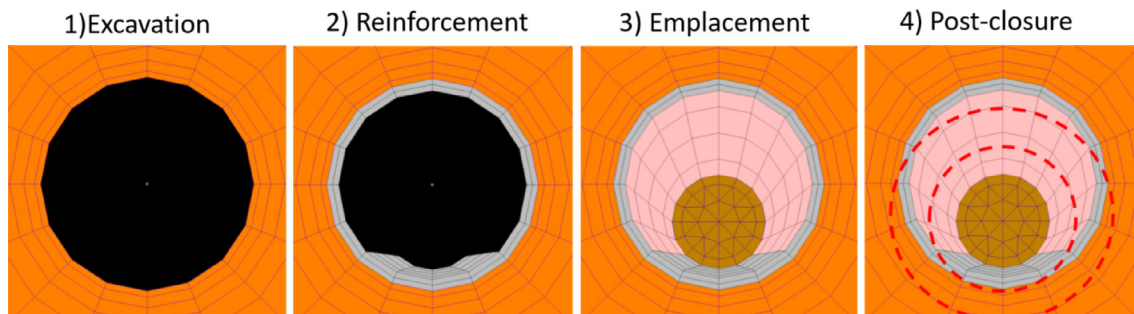


Fig. 2. Modeling steps: from tunnel excavation to post-closure period.

**Table 1**  
Basic THM properties of host rocks and concrete liner.

Parameter	Argillite (Opalinus Clay)	Crystalline (Granite)	Concrete
Bulk Density [kg/m <sup>3</sup> ]	2400	2700	2700
Porosity [-]	0.15	0.01	0.15
Young's Modulus [GPa]	5	35	23
Poisson's ratio [-]	0.3	0.3	0.2
Grain Specific heat [J/kg·°C]	900	900	900
Thermal conductivity [W/m·°C]	1.7	3.0	2.0
Thermal expansion coefficient [°C <sup>-1</sup> ]	$1.0 \times 10^{-5}$	$1.0 \times 10^{-5}$	$1.0 \times 10^{-6}$
Bulk Permeability [m <sup>2</sup> ]	$5.0 \times 10^{-20}$	$1.0 \times 10^{-17}$	$1.0 \times 10^{-19}$

**Table 2**  
Basic THM properties for the bentonite buffer representing FEBEX bentonite with simplification such a linear swelling and linear saturation dependent thermal conductivity (Rutqvist et al., 2011).

Parameter	Value/Function
Initial dry density, $\rho_d$ [kg/m <sup>3</sup> ]	$1.6 \cdot 10^3$
Initial porosity, $\phi$ [-]	0.41
Saturated permeability, $k$ [m <sup>2</sup> ]	$2.0 \cdot 10^{-21}$
Relative permeability, $k_r$ [-]	$k_{rl} = S_l^3$
Van Genuchten's (1980) parameter, $P_{VG}$ [MPa]	30
Van Genuchten's (1980) parameter, $\lambda_{VG}$ [-]	0.32
Thermal expansion, $\beta$ [1/°C]	$1.5 \cdot 10^{-4}$
Grain specific heat, $C_s$ [J/kg·°C]	800
Thermal conductivity, $\lambda_m$ [W/m·°C]	$\lambda_m = \lambda_{dry} + S_l \times (\lambda_{wet} - \lambda_{dry})$
Molecular diffusion coefficient, $D_{v0}$ [m <sup>2</sup> /s]	$2.16 \cdot 10^{-5}$
Mass flow times tortuosity factor, $\tau$ [-]	0.8
Bulk modulus, $K$ [MPa]	20
Poisson's ratio, [-]	0.35
Moisture swelling coefficient, $\beta_{sw}$	0.238

considering thermally engineered backfill material, i.e. a high heat conduction buffer material,  $\lambda_{dry} = 5$  W/mK and  $\lambda_{wet} = 10$  W/mK. These values are based on the recently published laboratory results by Chen et al., (2018) showing that thermal conductivity of bentonite could be increased by as much as an order of magnitude when using admixtures of graphene oxide. For example, by mixing with 30% graphene oxide,  $\lambda_{dry} = 5$  W/mK and  $\lambda_{wet}$  could be estimated to exceed 25 W/mK. In the model simulations, it is assumed that other properties of the bentonite are retained as the original FEBEX bentonite.

For initial conditions, hydrostatic fluid pressure and a thermal gradient of 28 °C per km are assumed. With the ground water table near the ground surface and a ground surface temperature of 10 °C, the initial pressure and temperature at 500 m depth is about 4.5 MPa and 24 °C, respectively. Isotropic stress field is assumed with the magnitude of the three principal stresses being equal to the weight of the overburden rock, leading to a slightly higher initial stress in the case of crystalline rock.

The modeling steps include excavation, reinforcement, emplacement of the waste canisters and buffer, followed by the post-closure simulation over 100,000 years (Fig. 2). It is assumed that the waste canister and buffer are installed at an instant defined as time zero in a post-closure simulations. The buffer is installed at an initial liquid saturation of 65%. Sevougian et al. (2019) developed several options of decay heat functions representative of existing and future inventories of DPCs on the basis of radionuclide inventories in Carter et al. (2013), including both 24-PWR and 37-PWR DPCs with a decay storage of up to 150 years before disposal (Table 3). In the model simulations performed here, the 24-PWR DPCs emplaced after 100 years-Out-of-the-Reactor (yOoR) is applied for the argillite disposal case, whereas the two optional 37-PWR DPC decay heat functions (emplaced at 100 and 150 yOoR) are applied for the crystalline host rock case. The decay functions for the 37-PWR DPCs are developed from Carter et al., (2013) considering fuel elements with of relatively high burn-up of 60 GWd/MTU (gigawatt-days/metric ton of Uranium), which results in a

relatively high initial decay heat. In Table 3, note the big difference in initial decay heat for 100 versus 150 yOoR, but at 1000 years the decay heat is almost the same and still above 1000 W. This is also clearly shown in Fig. 3, which presents the heat decay function in a linear time scale for the first 1000 years (Fig. 3a) and as a function of logarithm of time over 100,000 years (Fig. 3b). The initial decay heat is more likely to affect the early time peak temperature in the EBS, while the decay heat at 1000 years could have more impact on the more long-term temperature evolution of the system.

In the post-closure simulations, the geomechanical impact is evaluated in terms of the stress evolution at the repository level away from the emplacement tunnels as well as at the tunnel walls, where the stress concentrations are the highest. The stress-strain evolution is calculated considering linear poro-elasticity and thermo-elasticity, whereas the potential for failure is considered through stress criteria. For the repository level stresses, simple criteria is that tensile stress could induced tensile failure, while a shear stress equal to or larger than the shear strength could induced shearing of pre-existing fractures (Rutqvist et al., 2014). For the top and bottom of the emplacement tunnels, where the highest compressive tangential stress is expected to occur, a spalling failure criterion is considered through a uniaxial compressive strength. According to site investigations in hard crystalline (granitic) rock at the Manitoba underground research laboratory in Canada and at the Äspö hard rock laboratory in Sweden, a so-called spalling strength of about 120 MPa has been estimated (Andersson et al., 2009; Andersson and Martin, 2009; Martin and Christiansson, 2009; Rutqvist et al., 2009b). For the argillite case, a uniaxial compressive strength of 16 MPa is applied that is representative of laboratory determined values on Opalinus Clay (Corkum and Martin, 2007; Bock 2009; Rutqvist et al., 2014). On the sidewalls of the tunnel, there will be a relief of tangential compressive stress, which could potentially lead to development of tensile stress and tensile fracturing. Such geomechanical impact, being a results of the thermally driven coupled THM processes, will put limits on the maximum host rock temperature that can be tolerated, i.e. there will be an impact on the thermal management and design of the repository.

### 3. Conventional versus thermally engineered buffer

This section presents results of TH model simulations investigating the effects of using a buffer material that has been thermally engineered for high heat conduction. That is, to investigate how admixtures of high thermal conductivity materials to the bentonite could improve the thermal performance, by reducing the peak temperature in the buffer during the post-closure period. This is conducted for a repository in argillite host rock with a 24-PWR DPC, emplaced 100 yOoR. First, the basic and typical thermal-hydraulic responses considering conventional FEBEX bentonite are presented in Section 3.1. This is followed in Section 3.2 by a comparison to show the difference when considering a buffer that is thermally engineered for high heat conduction.



**Table 3**

Decay heat sources for various DPC packages and surface decay storage times. The data for the decay heat are derived from Carter et al., (2013).

DPC heat source name for the model	Burn-Up (GWd/MT)	Enrichment (%)	Number of PWR fuel elements per DPC	Surface Decay Storage Time (Years)	Decay Heat (Watts)	
					At disposal	1000 Years
24-PWR 50YOoR	40	3.72	24	50	7057	66
24-PWR 100YOoR	40	3.72	24	100	3881	64
37-PWR 100YOoR	60	4.73	37	100	8810	1224
37-PWR 150YOoR	60	4.73	37	150	5817	1179

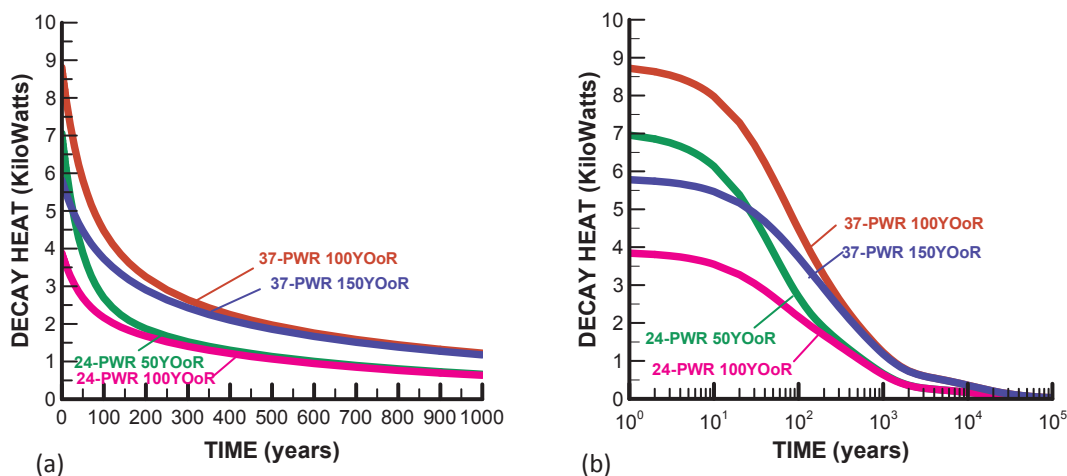


Fig. 3. Decay heat functions for various DPC packages and surface decay storage times displayed (a) over linear time to 1000 years, and (b) over logarithm of time to 100,000 years. The data for the decay heat are derived from Carter et al., (2013).

3.1. Conventional buffer material

Fig. 4 presents the evolution of temperature, buffer saturation and fluid pressure calculated for the case of a buffer material consisting of conventional FEBEX bentonite. Fig. 4a, shows that the temperature at the interface between the canister and buffer peaks at 150 °C within 10 years, and stays well above 100 °C for up to 1000 years (at Point V1 in Fig. 4a). The temperature at the rock wall (Point V2) peaks at 104 °C after 300 years, whereas the host rock temperature away from emplacement tunnels peaks at 85 °C after 750 years (Point V6). A significant drying takes place at the inner parts of the buffer during the first tens of year, and the buffer finally saturates fully after 75 years (Fig. 4b). The drying of the buffer near the canister is caused by evaporation and vapor diffusion along the thermal gradient across the buffer. Such drying has been observed at field heater experiments where a steep thermal gradient can cause very substantial drying (Alonso, 2005; Garitte et al., 2017b). This drying is later overcome by water inflow from the surrounding host rock that finally completely saturates the buffer after 75 years.

Fig. 4c shows that fluid pressure increases substantially, first in the host rock and then in the buffer. This is as a result of thermal pressurization, a phenomenon known to occur when heating pore-fluids in low permeability rocks, such as shale (Ghabezloo and Sulem, 2009; Gens et al., 2007; Rutqvist et al., 2014; Zhang, et al., 2017). Thermal pressurization is driven by temperature changes in the host rock away from the emplacement tunnel and peaks a few hundred years after the host rock temperature peaks. In this case, the weight of the overburden rock at 500 m depth results in 11.8 MPa vertical stress (lithostatic stress). The thermally driven increase in fluid pressure peaks at 14.6 MPa, which is several MPa higher than the vertical stress. This implies a significant risk for hydraulic fracturing of the host rock, which in reality should be avoided through appropriate design of the repository.

3.2. Thermally engineered buffer material

The potential benefits of a thermally engineered buffer material are investigated by comparison of simulation results for the thermally engineered high heat conduction bentonite with the results of conventional FEBEX bentonite. In Fig. 5, dashed lines are the results for the conventional FEBEX bentonite while solid lines are the results for the thermally engineered buffer material.

Fig. 5a shows that the peak temperature in the buffer at the canister surface reduces from 150 °C to 104 °C when using the high heat conduction buffer material. In the case of the high heat conduction buffer material, the thermal gradient across the buffer is also substantially reduced. This can be observed by the fact the temperatures at the canister (Point V1) and at the wall rock (Point V2) are not as different (red and blue solid lines in Fig. 5a). A reduced thermal gradient across the buffer has the benefit of preventing drying of the buffer next to the canister. For example, from Fig. 5b one can observe that in the case of conventional FEBEX bentonite properties, the water saturation decreases from 65% to 40% (dashed red line in Fig. 5b), while in the case of high buffer thermal conductivity, saturation decreases only a few percent (solid red line in Fig. 5b). The final time to full saturation is affected somewhat with a faster resaturation when using high thermal conduction bentonite, i.e. time to full saturation reduces from 75 to 60 years.

Another important observation in Fig. 5 is that the temperature evolution in the repository host rock is unchanged and does not depend on the thermal conductivity of the buffer (purple lines in Fig. 5a). In both cases, the temperature at the tunnel wall peaks at about 104 °C after 300 years, whereas the rock temperature away from the emplacement tunnel (Point V6) peaks at 85 °C after 750 years (Fig. 5a). Also, in both cases a very substantial increase in fluid pressure occurs as a result of thermal pressurization, with a pressure exceeding the lithostatic stress by several MPa (Fig. 5c).

In terms of thermal management and repository design, the results

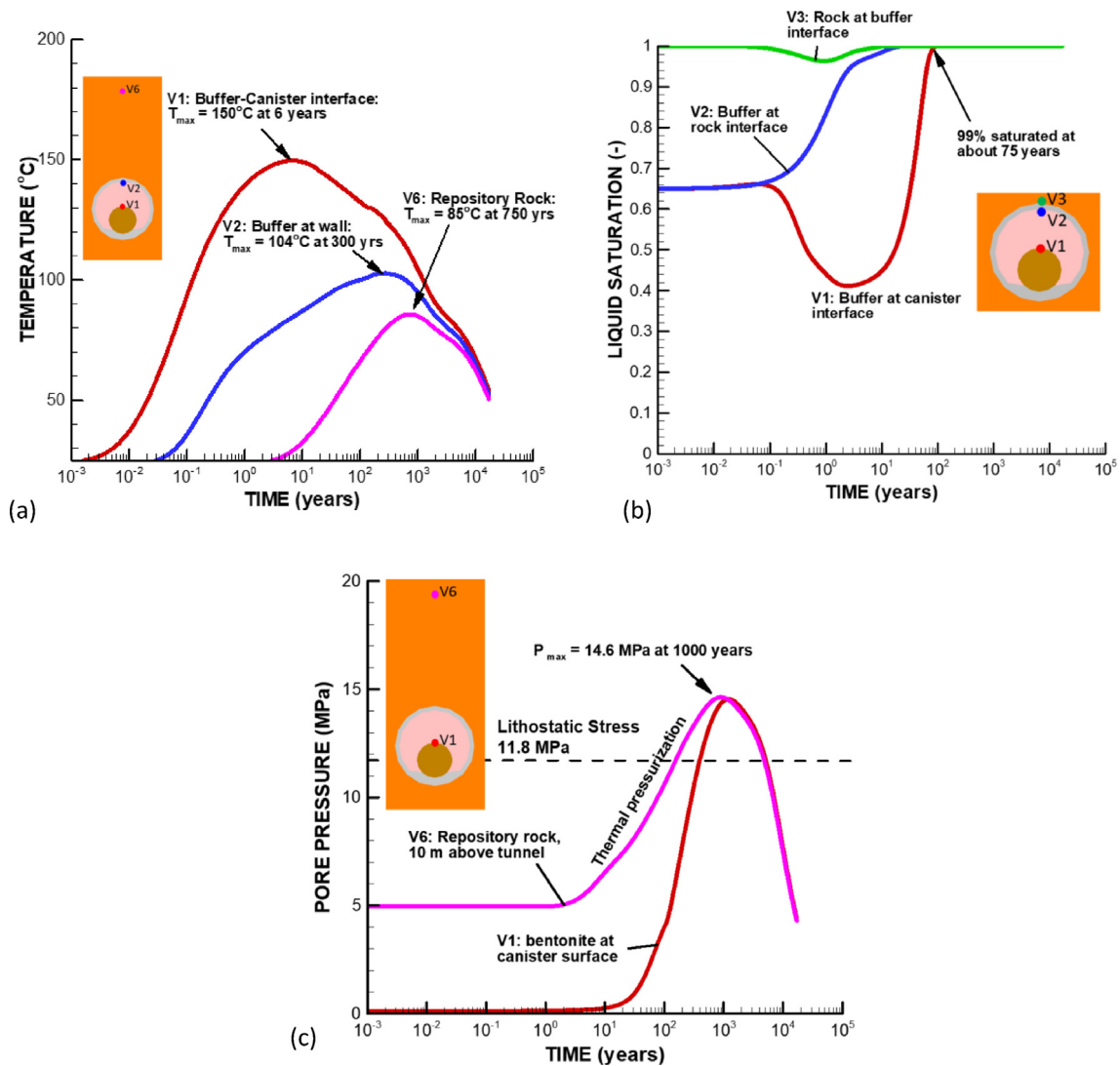


Fig. 4. Thermal-hydraulic simulation results for a repository in argillite considering a heat source from a 24PWR-100yOoR DPC and conventional FEBEX bentonite thermal conductivity: Evolution of (a) temperature, (b) saturation and, (c) pore pressure.

in Fig. 5 shows that peak temperature in the buffer can be substantially reduced using an engineered high heat conduction buffer material, while it does not significantly impact the host rock temperature. The impact of rock temperature changes on the coupled THM processes leading to geomechanical impact on the repository performance are investigated in the next section, for both argillite and crystalline host rocks.

#### 4. Host rock coupled thm responses

Thermally driven coupled THM responses in the host rock are investigated for a number of cases considering argillite (Opalinus Clay) and crystalline (granite) host rocks. In all cases, the repository emplacement tunnels are assumed to be located at 500 m depth with the same near-field geometry (Fig. 1), but in the case of a repository tunnel in argillite, a concrete liner is installed for reinforcement (Fig. 6). A thermally engineered, high heat conduction buffer is applied in all cases. However, as shown in Section 3, the thermal conductivity of the buffer does not significantly impact the temperature evolution in the host rock.

##### 4.1. THM response in argillite host rock with 24-PWR DPCs

Here the case of direct disposal of 24-PWR DPCs in argillite host rock is considered. The host rock temperature and pressure responses are those shown in Fig. 5 for the case of a thermally engineered, high heat conduction buffer. Fig. 7 presents the evolution of vertical and horizontal stresses at a point located 10 m above the emplacement tunnels (V6 in Fig. 1), and therefore, represents the general repository stress. In Fig. 7, both total and effective stresses are shown with the difference between the total and effective stresses being equal to the fluid pressure. The total vertical stress is approximately constant and equal to the weight of the overburden rock, which is about 11.8 MPa (Fig. 7a). The increase in the fluid pressure causes a reduction in the vertical effective stress, which becomes tensile at about 100 years. The tensile effective vertical stress lasts for several thousand years, and in reality this could cause tensile fracturing as previously mention. The horizontal total stress increases with the fluid pressure as a result of thermo-poro-elastic stress between the confined lateral boundaries (the model cannot expand in the horizontal direction and instead horizontal stress increases with increasing temperature and pressure). However, a strong reduction in vertical effective stress, which is the minimum principal stress causes a significant reduction in shear strength. Here the simple strength criterion applied implies that there is a potential for

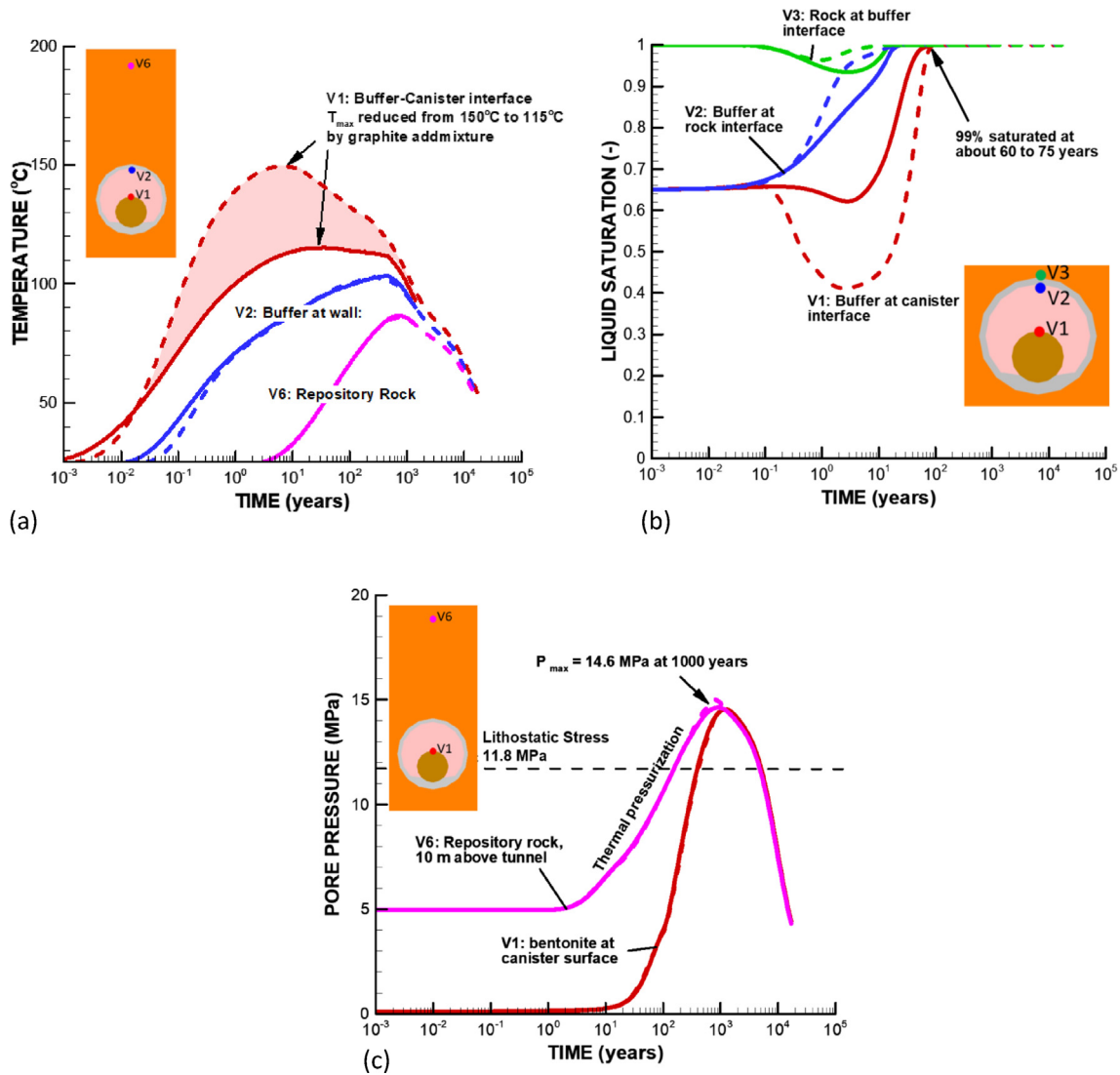


Fig. 5. Effect of thermally engineered bentonite buffer to enhance thermal conductivity and reduced peak temperature (heat source from a 24PWR-100yOoR DPC). Evolution of (a) temperature, (b) saturation and, (c) pore pressure. Dashed lines are the results for the conventional FEBEX bentonite thermal properties and solid lines are the results for thermally engineered high heat conduction bentonite.

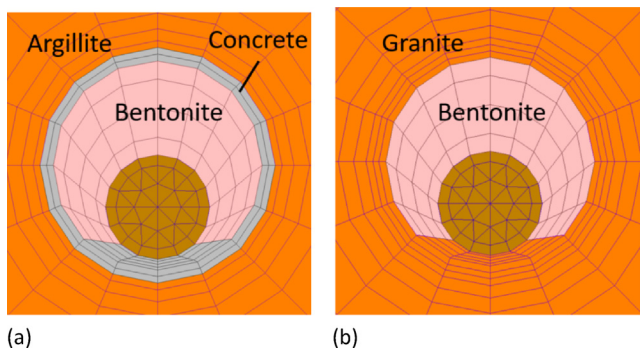


Fig. 6. Modeled EBS geometry for the cases of a repository tunnel located in (a) argillite (Opalinus Clay) and (b) crystalline (granite) host rock.

shear slip along existing fractures if the maximum compressive stress exceeds 3 times the minimum principal stress. This is based on a Mohr-Coulomb criterion assuming a coefficient of friction of 0.6 and zero cohesion and that fractures of any orientation could exist. In Fig. 7b, the blue shaded area is where the maximum compressive effective stress (horizontal stress) exceeds the shear strength and shear slip could occur

on existing fractures.

Figs. 8 and 9 present the evolution of stresses at the wall of the tunnel within the concrete liner (Fig. 8) and in the host rock just outside of the concrete liner (Fig. 9). After excavation and installation of the concrete liner, the stiffer concrete liner prevents further convergence of the softer argillite host rock, leading to a compressive tangential stress of up to 40 MPa within the concrete liner (Fig. 8). The radial stress is much smaller due to the free surface to the tunnel opening that is backfilled with bentonite of low initial stress. During the post-closure period, the tangential stress in the concrete liner is reduced, and a very high tensile effective stress occurs at the side of the tunnel (Fig. 8b green line). This high tensile stress would certainly cause tensile failure of the concrete liner that could potentially expand tensile failure out into the host rock. As mentioned, in these simulations, a linear elastic stress-strain behavior is considered and the potential for failure is evaluated by comparison to a stress criterion. In reality, if tensile failure occurs, the tensile stress could not increase as high as shown in Fig. 8b. The stress in the argillite host rock shown in Fig. 9 is smaller, though the magnitude of tangential stress is close to the uniaxial compressive strength of Opalinus Clay. However, the concrete liner provides confinement with a confining stress of several MPa, and therefore, rock failure may be minimal. The main concern with the results in Figs. 8

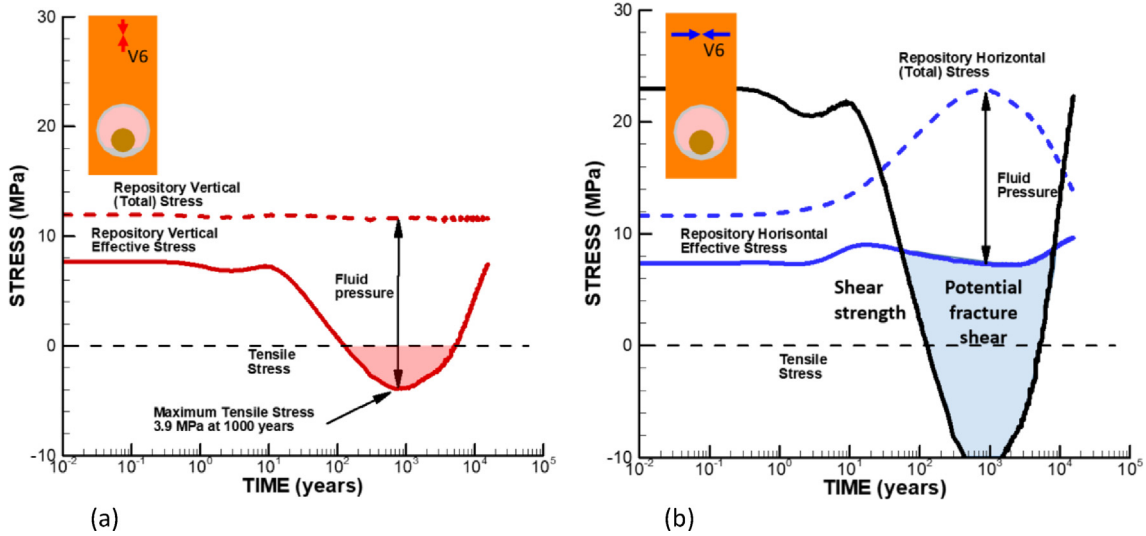


Fig. 7. Results of simulations of (a) vertical and (b) horizontal stresses for a repository tunnel in argillite and decay heat from a 24PWR-DPC emplaced at 100yOoR. Dashed lines are total stresses, and solid lines are effective stresses.

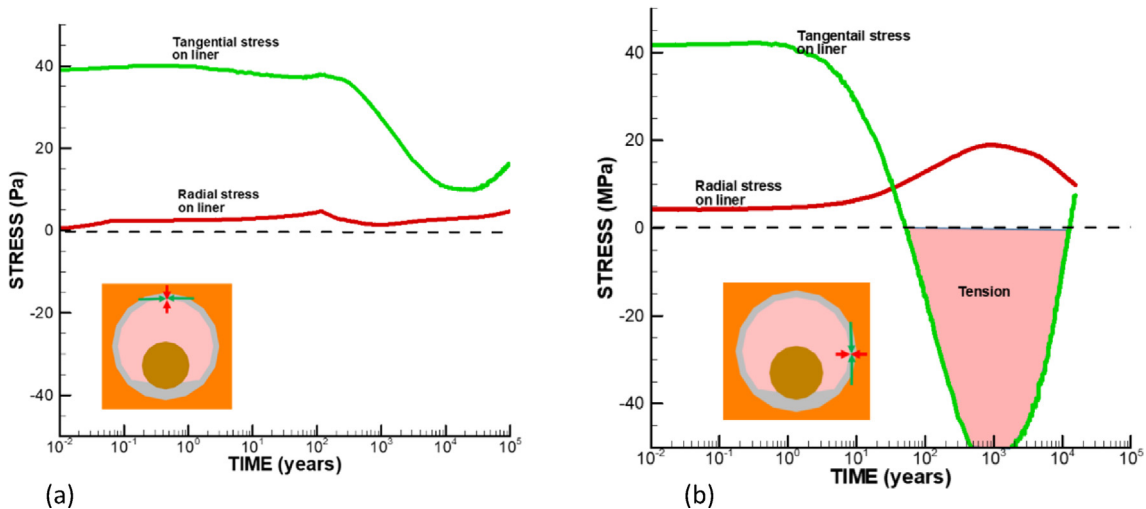


Fig. 8. Results of simulations of the evolution of stresses within the concrete liner: (a) at the top of the tunnel, and (b) at the side of the tunnel, for a repository tunnel in argillite and decay heat from a 24PWR-DPC emplaced at 100yOoR.

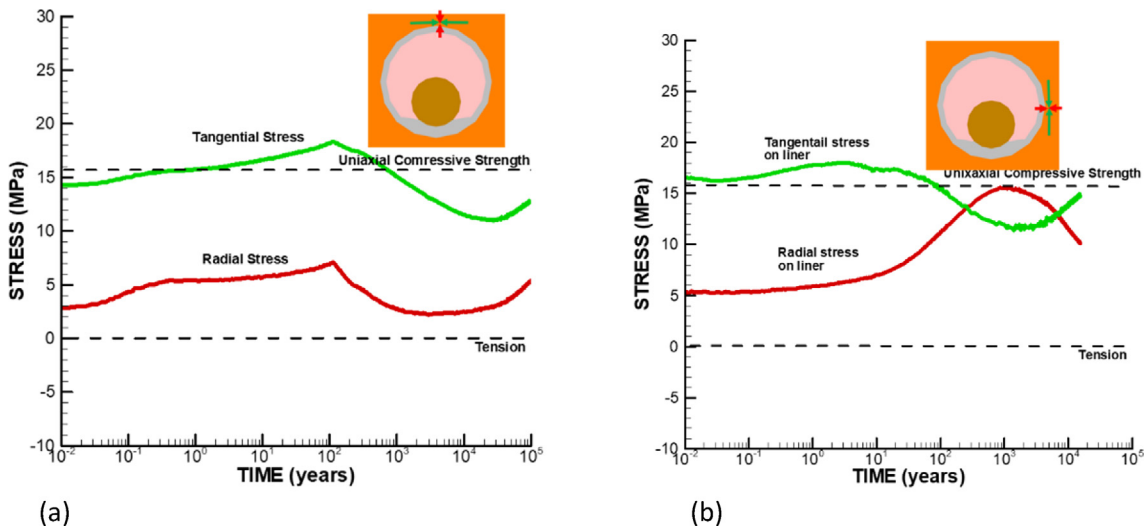


Fig. 9. Results of simulations of the evolution of stresses in the wall rock just outside the concrete liner: (a) at the top of the tunnel, and (b) at the side of the tunnel, for a repository tunnel in argillite and decay heat from a 24PWR-DPC emplaced at 100yOoR.



and 9, is the high tensile stress that would certainly create a tensile failure in the concrete liner and it would occur approximately 100 years after emplacement. However, at 100 years, the buffer is fully saturated with fully developed swelling stress, meaning that any voids created by such fracturing of the liner would likely be invaded and sealed by the swelling bentonite.

4.2. THM response in fractured granite with 37-PWR DPCs

Compared to the argillite, the fractured granite is much more permeable and stiffer, which makes the coupled THM responses different, including less pronounced thermal pressurization and more pronounced thermal stress. Moreover, the thermal conductivity of the granite is 3.0 W/mK, which is almost twice as high as that for the argillite host rock (Table 1). Here two cases are tested to demonstrate the effect of surface storage for thermal decay on the thermal management and coupled THM responses: (1) 37-PWR elements with disposal at 100 yOoR and (2) 37-PWR elements with disposal at 150 yOoR (Table 3). The higher initial decay heat for 37-PWR element DPCs compared to 24-PWR element DPCs, can be applied in the case of granite considering the same repository design and geometry, because of the twice as high rock thermal conductivity.

The results for the two cases of 37-PWR DPCs, emplaced at 100 and 150yOoR are presented in Figs. 10–12. Despite a very high decay heat from the 37-PWR DPCs, the peak temperatures are rather moderate, up to 135 °C for the case of emplacement at 100yOoR (Fig. 10a). Here the peak temperature within the buffer is effectively kept relatively low, because of the thermally engineered high heat conduction buffer in combination with the relatively high thermal conductivity of the granite host rock. The peak temperature at the buffer/wall is lowered from 135 °C to about 120 °C if the emplacement is delayed from 100 to 150yOoR, which is not a dramatic decrease. Both 135 °C and 120 °C are temperatures well below a 150 °C criterion for potential changes in bentonite swelling properties, though higher than the stringent 100 °C limit enacted in for example the Swedish nuclear waste program. The peak temperature in the host rock is lowered by just 10 °C, from about 120–110 °C, showing that longer surface decay storage have rather small impact on the longer term host rock peak temperature. In fracture crystalline rock, thermal pressurization is not strong as shown in Fig. 10b, because any increase in pore pressure can quickly diffuse because of the relatively high rock permeability.

The rock stress evolution at the repository level (as shown in Fig. 11) for fractured granite is quite different from that in argillite (as

shown in Fig. 7). The main geomechanical response for the fractured granite case is an increase in the horizontal stress caused by thermal stress due to temperature changes in the host rock. An increase in the horizontal stress, while vertical stress is approximately constant, causes an increase in differential (shear) stress. If the shear stress is sufficiently large, shear activation of pre-existing fractures and/or faults could occur, in particular for fractures that are optimally oriented for shear activation in the disturbed stress field.

The shear strength calculated as 3 times them minimum compressive principal stress is starting at about 28 MPa, and then decreases to less than 20 MPa at about 10 years (Fig. 11b). The horizontal compressive stress exceeds the strength from about 10 years, and remain high for up to 10,000 years. High shear stress prolonged for such a long time in a fractured rock mass has the potential for inducing fracture shear activation.

The increasing host rock horizontal thermal stress will cause even stronger stress changes at the tunnels walls as shown in Fig. 12. At the top of the tunnel, the compressive stress to increase and peak at 128 MPa after about 6000 years for the case of 37PWR 100yOoR. Such a high compressive tangential stress is close to the spalling strength observed at excavations in granite at the Äspö Hard Rock Laboratory (Andersson et al., 2009; Andersson and Martin, 2009; Martin and Christiansson, 2009). However, those values are for unsupported tunnel walls, whereas in this case a support stress has already developed by the swelling stress in the buffer. As observed in Fig. 12a, the radial stress has increased to about 5 to 10 MPa, and therefore, the tangential stress of 128 MPa would not likely induce any significant damage to the host rock. At the side of the tunnel, the stresses are relatively small, but with some potential for tension in the tangential stress (Fig. 12b).

5. Discussion

This study provides new insight into thermal management associated geologic disposal of large disposal canisters, such as dual purpose canisters evaluated for disposal in the U.S. DOE nuclear waste disposal research. Importantly, the study demonstrates the feasibility of disposal of very large sized nuclear waste canisters in bentonite-backfilled tunnels. This can be accomplished by the use of bentonite engineered for high heat conduction, such that the high amount of decay heat from large disposal canisters can be efficiently transferred into the surrounding host rock. The way this works is further illustrated in Fig. 13, comparing the distributions of temperature and saturation at 10 years after emplacement of the canister. With a buffer thermally engineered

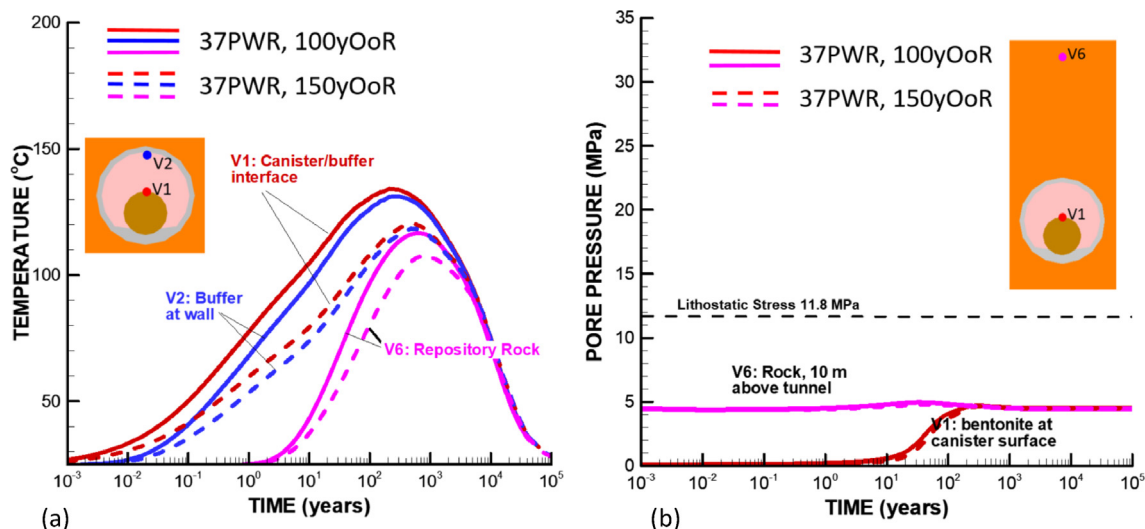


Fig. 10. Results of simulations of (a) temperature, and (b) pore pressure, demonstrating the impact of surface heat decay storage time (disposal at 100 or 150yOoR for a 37PWR DPC) on the thermal-hydraulic response for a repository tunnel in fracture granite.

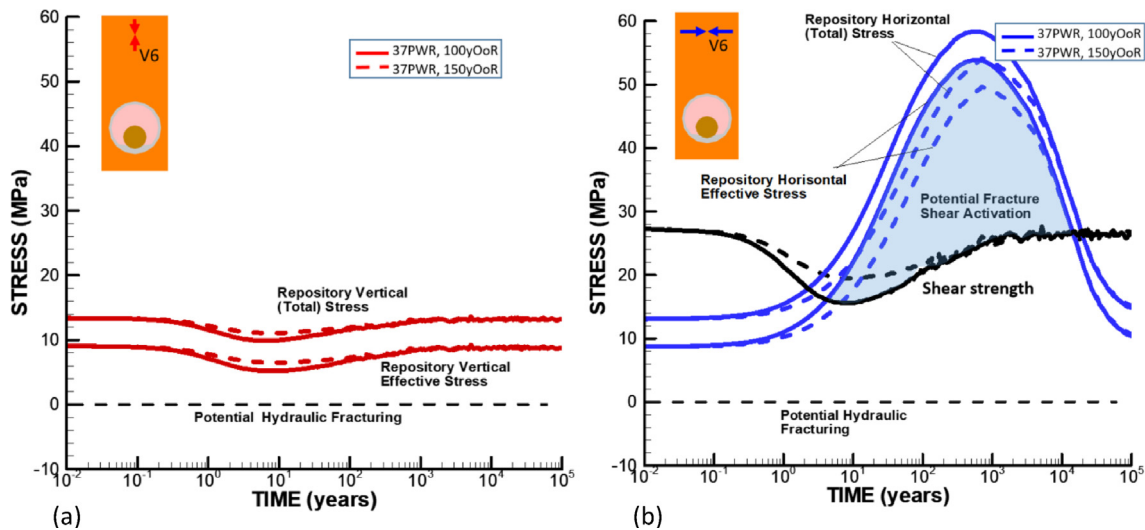


Fig. 11. Results of simulations of (a) vertical, and (b) horizontal stresses for a repository tunnel in fractured granite and decay heat from a 37PWR-DPC emplaced at 100 or 150yOoR.

for high heat conduction, the heat can be effectively transferred to other parts of the bentonite buffer and then released into the surround host rock (Fig. 13a). The much reduced thermal gradient across the buffer do also eliminate evaporation drying (and any potential desiccation fractures) near the waste canister and this can actually accelerate the re-saturation and swelling of the buffer (Fig. 13b). It is important to develop a swelling stress to assure the protective function of the buffer and eliminate any voids that otherwise could host microbial activities.

This study also demonstrates the importance of the far-field repository temperature in creating thermal stress and thermal pressurization that if not managed could lead to wide-spread fracturing or shear activation of fractures and faults, as well as high stress concentration and damage around emplacement tunnels (Fig. 14). Because the vertical stress remain constant and equal to the weight of the overburden, thermally-induced horizontal stress will result in an increased shear stress that will be the driver for potential activation of fractures and faults (Fig. 14a). Such shear activation could result in an increased permeability and could also potentially induce small seismic events. Finally, the increasing horizontal stress will act on the repository tunnels and that through stress concentration around the tunnel openings could cause compressive spalling failure or tensile failure to different parts of the tunnel walls (Fig. 14b). These are

thermally-induced coupled THM processes that need to be evaluated in the thermal management of a nuclear waste repository over a post-closure period of up to 100,000 years.

A further step would be to estimate potential consequences if thermally induced irreversible geomechanical changes occur. This would include both the magnitude and distribution of shear and tensile failure in a full elasto-plastic analysis, perhaps including discrete fracture model approaches (Min et al., 2004; Hu et al., 2017; Hu and Rutqvist, 2020). For example, a massive shear activation of a well-connected fracture network in crystalline rock could enhance permeability by several orders of magnitude based on field observations in fractured rocks (Rutqvist and Stephansson 2003; Min et al., 2013; Rutqvist, 2015). In soft and ductile argillite, permeability changes with fracture shear is not obvious and fractures might seal quickly after the shear (Nguyen et al., 2019). The potential for induced seismicity and the potential magnitude of such an event will depend on the shear stress drop during the shear activation and the size of the rupture area (Urpil et al., 2019). In the case of crystalline rock, more brittle shear slip could be expected and therefore there could be a potential for inducing seismic events that could be felt on the ground surface (Yoon and Zang, 2019). Considering recent issues and public concern with induced seismicity associated with underground injection activities (Ellsworth,

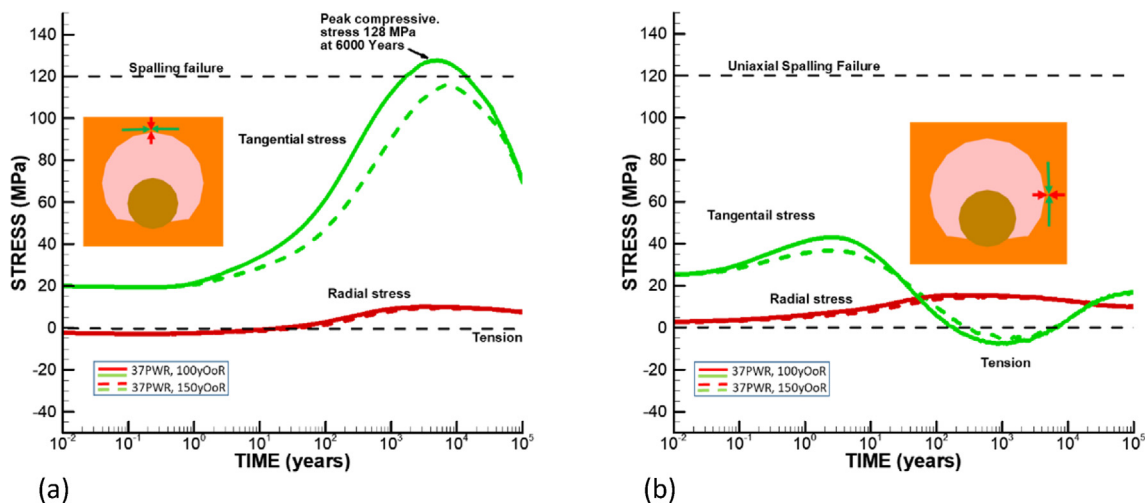


Fig. 12. Results of simulations of stresses in the wall rock: (a) at the top of the tunnel, and (b) at the side of the tunnel, for a repository tunnel in fractured granite and decay heat from a 37PWR-DPC emplaced at 100 or 150yOoR.

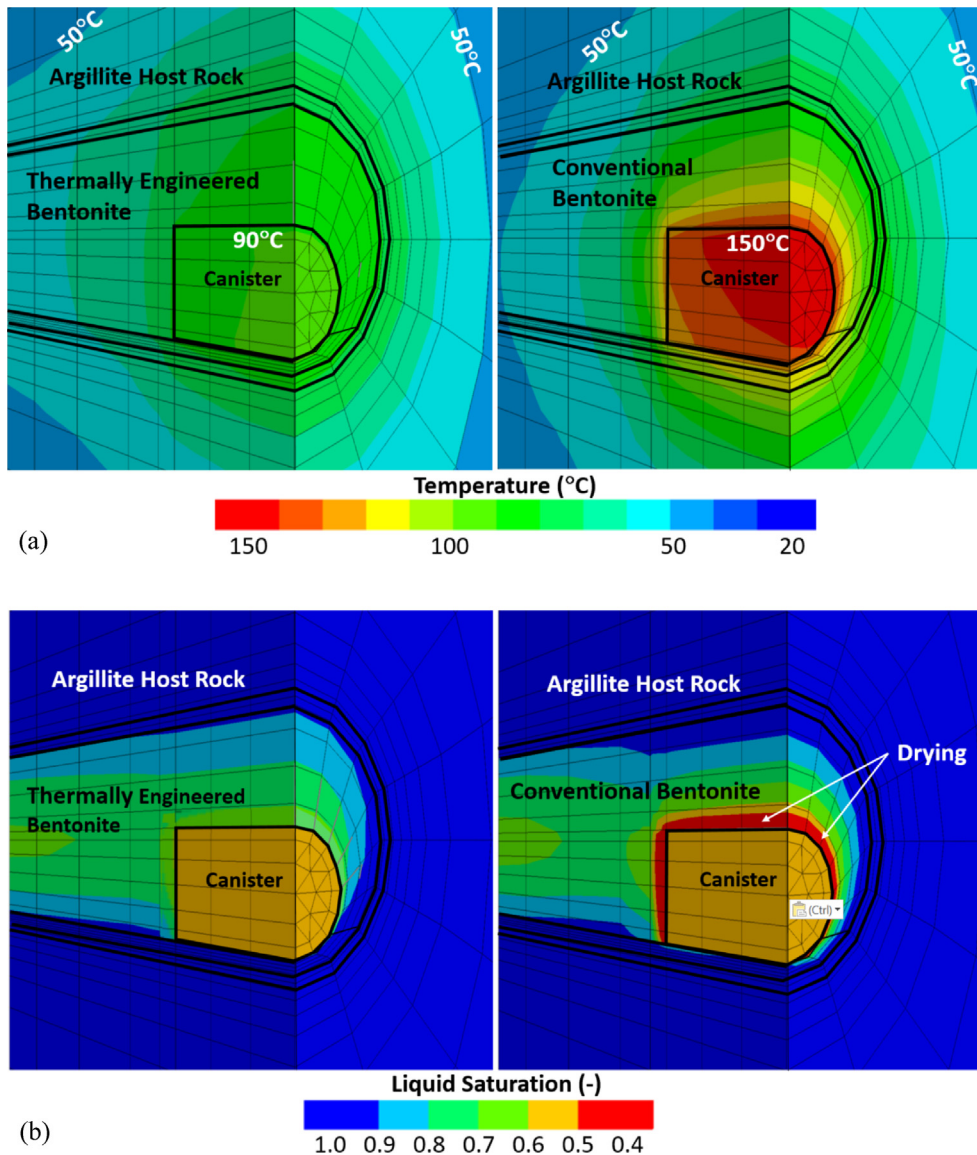


Fig. 13. Calculated (a) temperature and (b) liquid saturation 10 years after emplacement for thermally engineered (left) and conventional bentonites (right) for a repository tunnel in argillite and decay heat from a 24PWR-DPC emplaced at 100yOoR.

2013; McGarret et al., 2015; Grigoli et al., 2018), the potential induced seismicity associated with nuclear waste disposal needs to be evaluated, especially associated with disposal of large sized disposal canisters.

The potential for thermally-induced damage and permeability enhancement in the EDZ around tunnels has been studied in field experiments in both crystalline and argillite host rocks, such as at the Äspö Hard Rock Laboratory in Sweden for crystalline rock (Andersson et al., 2009; Hudson et al., 2009; Martin and Christiansson, 2009) and at the Mont Terri Laboratory in Switzerland for argillite (Blümling et al., 2007; Kim et al., 2020). At both locations, the important function of the backfill to provide confinement to the excavation walls has been demonstrated. At the Äspö Hard Rock Laboratory it was found that a small confining stress supporting the excavation wall would be sufficient to prevent thermally induced spallation (Andersson et al., 2009). Similarly, at Mont Terri, it was found that a 2 MPa stress would be sufficient to seal fractures and thus effectively reduce the permeability of the EDZ (Blümling et al., 2007). This again highlights the importance of a timely resaturation and swelling of the bentonite backfill, which as shown in this study, can be accelerated by the use of thermally engineered, high heat conduction backfill.

Finally, it is acknowledged that the current study of thermally

engineered backfill is a first attempt considering just published thermal laboratory experimental data. The backfill thermal conductivity was assigned a very high thermal conductivity based on recent experimental results on bentonite mixed with graphene oxide (Chen et al., 2018). Bentonite mixed with other minerals such as graphite or quartz sand have also shown to increase thermal conductivity, but not as much (Jobmann and Buntebarth, 2009; Chen et al., 2018). Further studies are desirable, including both laboratory and in situ heating experiments with bentonite engineered for high heat conduction. If successful, thermally engineered backfill could be an important future direction to enable disposal of large sized waste canisters even in bentonite-backed emplacement tunnels, without overheating and thermally degrading the protective functions of the buffer.

## 6. Conclusions

Overall, the study highlights the fact that a proper design of the Engineered Barrier System (EBS) can be applied to reduce the buffer peak temperature to acceptable levels, whereas the longer term far field host rock temperature evolution can still be a critical parameter that must be considered in the thermal management and design of a nuclear



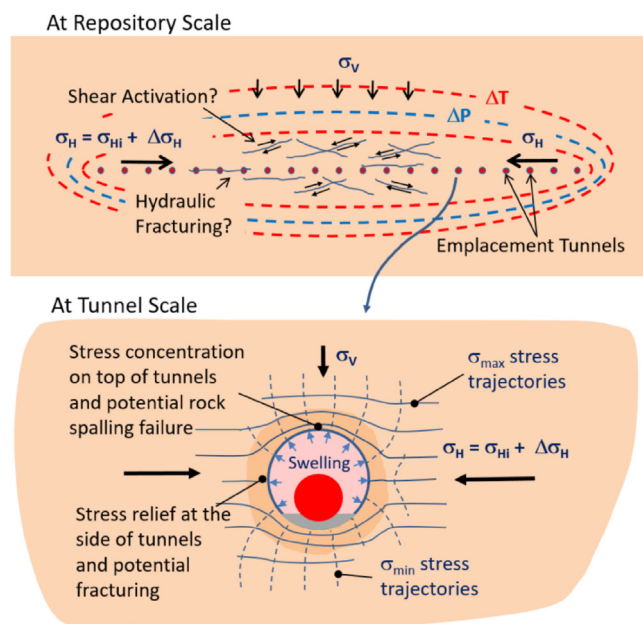


Fig. 14. Schematic of repository scale coupled thermo-hydro-mechanical responses and their impact on emplacement tunnels.

waste repository. Specific findings are as follows:

- The peak temperature in the buffer can be reduced below acceptable levels if the EBS, including the backfill/buffer is engineered for high heat conduction to effectively transfer the heat released from the waste canisters through the buffer and into the surrounding host rock.
- For a repository in argillite, the simulations show that thermal pressurization in the host rock is an important coupled process to manage as the fluid pressure could potentially exceed the lithostatic stress and thereby induce hydraulic fracturing and/or fracture shear activation. The thermal pressurization is driven by the overall repository temperature in the host rock, which may peak about 1000 years after closure of the repository. The thermal pressurization also results in an increase in horizontal stress that in turn increases repository shear stress and concentration stress around emplacement tunnels.
- For a repository tunnel in crystalline rock, thermal stress in the host rock is of greatest concern, as the induced horizontal thermal stress can cause shear activation of fractures in the host rock as well as spalling and tensile failure around emplacement tunnels. The thermal stresses that may peak several thousand years after emplacement and closure of the repository, could cause unwanted changes in permeability and may have the potential for inducing small seismic events.
- Thermal engineering of the bentonite buffer for high heat conduction can be further beneficial for the repository performance. With high thermal conduction bentonite, the thermal gradient across the buffer is minimized, which effectively reduces evaporation-drying near the waste canister. This is beneficial for assuring a timely re-saturation and the development of a uniformly distributed buffer swelling to maintain the protective functions of the buffer and tightness of the EBS.

Backfill material engineered for high thermal conductivity could be important for managing the near-field temperature in nuclear waste disposal, especially for disposal of large nuclear waste canisters such as the dual purpose canisters considered in this study. It may enable the disposal of large spent nuclear fuel canisters into a multi-barrier repository with bentonite backfill, which could be a safe disposal

solution. Finally, thermal management and repository design must always consider thermally driven coupled THM processes in the host rock with the peak impact that may occur thousands of year after repository closure.

## Acknowledgement

This work was supported by the Spent Fuel and Waste Science and Technology Campaign, Office of Nuclear Energy, of the U.S. Department of Energy under Contract Number DE-AC02-05CH11231 with Lawrence Berkeley National Laboratory.

This is a technical paper that does not take into account contractual limitations or obligations under the Standard Contract for Disposal of Spent Nuclear Fuel and/or High-Level Radioactive Waste (Standard Contract) (10 CFR Part 961). For example, under the provisions of the Standard Contract, spent nuclear fuel in multi-assembly canisters is not an acceptable waste form, absent a mutually agreed to contract amendment.

To the extent discussions or recommendations in this paper conflict with the provisions of the Standard Contract, the Standard Contract governs the obligations of the parties, and this paper in no manner supersedes, overrides, or amends the Standard Contract.

This paper reflects technical work which could support future decision making by DOE. No inferences should be drawn from this paper regarding future actions by DOE, which are limited both by the terms of the Standard Contract and a lack of Congressional appropriations for the Department to fulfill its obligations under the Nuclear Waste Policy Act including licensing and construction of a spent nuclear fuel repository.

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