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Implications of thermally-induced fracture slip and permeability change on the long-term performance of a deep geological repository

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1. Introduction

Radioactive wastes must be contained and isolated from people and the environment for a very long time. Disposal of these wastes to deep underground repositories in suitable geological formations is being developed by many countries worldwide [1,2]. The intention of such disposal is to provide sufficient isolation, both from human activities and from natural processes, such that the transport of radioactive nuclides in the geosphere will be a very slow process and their eventual release to the biosphere will be in such low concentrations that they pose no threat to human health or the natural environment. To that end, the repository must be designed in such a way that there can be an extremely high level of confidence that it can function as a barrier between nuclear waste and the environment for as long as 100,000 years. Fulfilling such a strenuous criterion successfully is what distinguishes geological repositories from other underground, engineering facilities [2]. An important aspect of the performance and safety assessment of disposal systems for radioactive waste and spent nuclear fuel in deep geological formations is to evaluate the combined effects of mechanical deformation, groundwater flow through the repository, and thermal loading from the decaying waste on the performance of the repository [3].

In a geological repository, excavation of a repository tunnel and deposition holes, along with the thermal stress generated from heat-generating nuclear waste, are the main factors that contribute to alteration of the stress state. The effect of excavation is expected to develop in the near-field - that is defined to be within a distance that is a few times the diameters of the repository tunnel and deposition holes. On the contrary, the influence of thermal stress will reach far-field areas, which can range from tens of meters to a few hundred meters from the periphery of the repository. The excavation damage zone is created in the near-field, and its potential for changing the permeability of the rock formation has been an issue of great concern in various candidate rock formations [4–6].

Thermal stress, which is the main factor that affects the stress state, is generated due to the confined nature of the rock. It is important to note that thermal stress is generated predominantly in a horizontal direction because the surface of the ground is unconfined. This thermal stress will be generated beyond the near-field of the repository, and the resulting high thermal stress ratio generally will act in favor of shear slip and dilation in the geological repository [7]. The phenomenon of shear displacement and dilation of fractures due to thermal loading is termed ‘thermoshearing’, and, since the dilated fractures will become the major pathway for fluid flow in the fractured rock mass, it is vitally important that the mechanisms of this phenomenon be studied and understood to ensure the safe disposal of nuclear waste in deep underground repositories. A field investigation by Barton...
et al. [8] indicated it is the critically stressed fractures that carry the major portion of the fluid flow, and this finding was also numerically demonstrated by Min et al. [9]. While characterizing permeability is one of the most important tasks in determining the feasibility of a deep geological repository for nuclear waste, it is important to recognize that the fluid-carrying ability of underground rock, i.e., its permeability, is a dynamic variable during the lifespan of a geological repository [10]. Another important consideration is that the thermoshearing and the resulting changes in permeability may not be reversible when the nuclear waste cools, because numerous fractures within the rock mass will undergo irreversible deformations during the heating phase [4,11].

While various mechanisms have been investigated to explain the processes that cause permeability to change under normal and shear stress [12–14], the effect of mechanical stress on permeability in the context of a geological repository has been found to be confined mainly to the near-field scale around the deposition holes or tunnels [15,16]. It was shown that multiple locations around the near-field can undergo shear slip along discontinuities due to excavation and thermal stress. This potential shear slip may induce increased permeability, which can then affect the calculation of radionuclide transport [17]. Also, these studies of the combination of the thermal, hydraulic, and mechanical effects were conducted in a deterministic manner, while the possibility of changes in permeability must be assessed by a probabilistic approach due to the uncertainty involved in the characterization of the discrete fracture network.

This paper addresses thermally-induced shear slip, i.e., thermoshearing, and changes in permeability of a deep geological repository in large scale. The geological data used for this analysis were acquired at the Forsmark site in Sweden, which was chosen as a candidate site by the Swedish Nuclear Fuel and Waste Management Company (SKB) after 7 years of site assessment [18]. The Swedish method for the development and use of a deep geological repository to isolate high level nuclear waste is the KBS-3 concept which involves encapsulating the waste in copper canisters with cast iron inserts and then embedding the canister, surrounded by bentonite clay, in the bed rock at a depth of about 400–500 m. The safety of such a repository will be assured by the performance of the natural and engineered barriers that act to prevent or delay the transport of radioactive nuclides to the biosphere [18]. The Forsmark site seems to have a high stress ratio (the ratio of major principal stress to minor principal stress), and this implies that many fractures at the site are critically stressed or almost so under the current stress state. Thus, even a slight change of stress can trigger a shear slip.

First, we present in this paper a systematic examination of the thermal stress expected to be generated in the far-field around the repository throughout its operation. Second, we present the results of a probabilistic shear slip analysis that was conducted based on the thermal loading history around the repository in order to investigate the possibility of thermoshearing. Third, we present the results of numerical experiments conducted on an explicitly-generated fracture network to quantify the change and irreversibility of permeability in the rock surrounding the repository.

2. Methodology and geological data

2.1. Methodology

This study was composed of the three steps. In the first step, a three-dimensional, thermo-mechanical analysis was conducted to obtain a full stress history in the far-field around the repository. For the analysis, we used a flexible, partial differential equation solver, COMSOL MULTIPHYSICS, which uses the finite-element method [19]. For this study, a calculation scheme for thermoelastic stress was implemented by incorporating the strain due to thermal expansion. The sizes of the models were 2 km x 2 km x 0.8 km (height) and 600 m x 600 m x 13 m (height) for the regional and repository scales, respectively. The analysis up to 10,000 years after deposition was expected to identify the potential for shear slip to occur in the far-field areas of the repository. Although no great technical hurdles were encountered in modeling thermal stress, systematic examination of this phenomenon is lacking in the pertinent literature. In the second stage, the quantitative analysis for shear slip potential was conducted in selected locations. The probability of the occurrence of shear slip at a fracture was examined by the Mohr-Coulomb failure criterion. The fracture orientations were generated stochastically based on statistical data from fracture mapping at the site, and the stress history obtained from the first stage was used. The probability of shear slip was calculated by dividing the number of fractures that failed by the total number of fractures. Finally, the stress history obtained from the first stage was used as the boundary conditions using the Discrete Fracture Network-Discrete Element Method (DFN-DEM) approach [9]. Based on the site investigation, the DFN was constructed at selected points [18]. In this study, it was possible to quantify the extent of shear dilation under the specific stress state and the nature of the irreversibility of permeability through the application of stress release expected to occur after the spent fuel cools. Generic data for the stress-transmissivity relationship for a single fracture were used. The two-dimensional, distinct-element code, UDEC, was used for the DEM calculation in this study [20].

2.2. Probabilistic shear-slip analysis

Given the orientation of a fracture and the stress field, normal and shear stress acting on the fracture plane can be determined. To evaluate the probability of shear slip at generated fractures, we used the Mohr-Coulomb failure criterion, assuming zero cohesion, as follows:
\[
\tau = \mu \sigma
\]

(1)

where \( \tau \) is shear stress, \( \sigma \) is normal stress, and \( \mu \) is the coefficient of friction. According to this failure criterion, shear slip occurs if shear stress is greater than the normal stress multiplied by the coefficient of friction. When a stress field is defined by a stress tensor, we can calculate the stress vector acting on a plane with a normal vector by Cauchy’s formula in order to evaluate against the failure criterion [21].

Two types of data sets for fracture orientations were used in this study. The first type of data set, random orientations, was generated based on a probability distribution function (PDF) with a uniform distribution of orientation. The second type of data set was chosen as a site-specific study based on the fracture data from the site investigation at Forsmark, Sweden as listed in Table 1 [22].

The probability of shear slip was calculated by the generation of random or distributed fractures. The Latin hypercube sampling (LHS) method was used for the generation of fractures [23]. The LHS method is similar to the Monte Carlo method in that it is used to select \( n \) different values from each of \( k \) variables. However, because the Monte Carlo method randomly selects \( n \) different values based on the probability of a cumulative distribution function (CDF), this method yields reasonable values only if the value of \( n \) is quite large. Thus, in order to increase the efficiency of the sampling method, the LHS method made selections in each of the non-overlapping intervals based on the equal probability of CDF, which provided reasonable values even when the value of \( n \) remained relatively small. In addition, the values of \( n \) associated with certain variables were paired with the values of \( n \) associated with other variables in a random manner until an \( n \times k \) matrix was formed.

In each case of random and actual fracture orientation, 10,000 samples were generated. Since we assumed that the four fracture sets had the same density, we generated 2500 samples for each set. In order to generate fracture orientations and calculate the probability of shear slip, a program was developed that generated the fracture orientation and then conducted a probabilistic analysis of shear slip.

2.3. DFN-DEM analysis

The DFN-DEM analysis used the discrete fracture network (DFN) as the geometry of the fractured rock and applied the discrete element method for the analysis of the mechanical and hydraulic behavior [9,24]. Two steps are involved in the hydro-mechanical analysis, i.e.,

<table>
<thead>
<tr>
<th>Fracture Set</th>
<th>Fracture orientation</th>
<th>Fracture size</th>
<th>Fracture intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trend (mean)</td>
<td>Plunge (mean)</td>
<td>Fisher ( \kappa ) (mean)</td>
<td>Minimum radius ( r_0 ) (m)</td>
</tr>
<tr>
<td>NE</td>
<td>314.9</td>
<td>1.3</td>
<td>20.9</td>
</tr>
<tr>
<td>NS</td>
<td>270.1</td>
<td>5.3</td>
<td>21.3</td>
</tr>
<tr>
<td>NW</td>
<td>230.1</td>
<td>4.6</td>
<td>15.7</td>
</tr>
<tr>
<td>SH</td>
<td>0.8</td>
<td>87.3</td>
<td>17.4</td>
</tr>
</tbody>
</table>

Table 1
Rock fracture statistics [22].

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m(^3))</td>
<td>2700</td>
</tr>
<tr>
<td>Elastic modulus (GPa)</td>
<td>70</td>
</tr>
<tr>
<td>Poisson's ratio (rock mass)</td>
<td>0.24</td>
</tr>
<tr>
<td>Thermal expansion coefficient (°C)</td>
<td>7.7 x 10(^{-6})</td>
</tr>
<tr>
<td>Specific heat (J/kg/°C)</td>
<td>796</td>
</tr>
<tr>
<td>Friction angle (deg)</td>
<td>37</td>
</tr>
<tr>
<td>Normal stiffness (GPa/m)</td>
<td>656</td>
</tr>
<tr>
<td>Shear stiffness (GPa/m)</td>
<td>34</td>
</tr>
<tr>
<td>Dilation angle (deg)</td>
<td>3.2</td>
</tr>
<tr>
<td></td>
<td>At the 20-MPa stress level</td>
</tr>
</tbody>
</table>

Table 2
Rock and fracture properties from Forsmark used in this study [18]. It is noted that only representative rock and fracture domains were selected from the site investigation.
application of boundary stress for mechanical calculation and (2) application of hydraulic pressure to determine the equivalent permeability at the given stress level. The details of the calculation methods are presented in [9,24]. The merit of this analysis is that the effect of stress can be investigated readily by changing the stress conditions through repetition of the numerical experiments. The stress values used in this study came from the sum of the thermal stress generated in the thermo-mechanical analysis and the measured in-situ stress. Reference points were selected to trace the change of resultant stress and these stresses were used subsequently as boundary conditions.

2.4. Geological data

The geological data used in this study were based on the site investigation at Forsmark that has been conducted by SKB [18]. The properties of the intact rock and the fractures for the DEM calculation are listed in Table 2. A linear stiffness model was used for the DEM calculation to simplify the stress-aperture change relationship. The elasto-plastic analysis used in this study ensured that the shear slip and corresponding dilation could be modeled properly as stress changes. The failure criteria used in this study were the Mohr–Coulomb criteria with zero cohesion. The initial and residual ap-

<table>
<thead>
<tr>
<th>In-situ stress</th>
<th>Vertical</th>
<th>0.0265z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minor horizontal</td>
<td>11.0+0.006z (z&lt;150 m)</td>
<td></td>
</tr>
<tr>
<td>Minor horizontal</td>
<td>6.8+0.034z (150 m&lt;z&lt;400 m)</td>
<td></td>
</tr>
<tr>
<td>Minor horizontal</td>
<td>9.2+0.028z (400 m&lt;z&lt;600 m)</td>
<td></td>
</tr>
<tr>
<td>Major horizontal</td>
<td>19.0+0.008z (z&lt;150 m)</td>
<td></td>
</tr>
<tr>
<td>Major horizontal</td>
<td>9.1+0.074z (150 m&lt;z&lt;400 m)</td>
<td></td>
</tr>
<tr>
<td>Major horizontal</td>
<td>29.5+0.023z (400 m&lt;z&lt;600 m)</td>
<td></td>
</tr>
</tbody>
</table>

In-situ temperature

6.0−0.012z

ertures were 70 mm and 10 mm, respectively, based on the previous study [24].

3. Far-field thermo-mechanical analysis of a KBS-3-type repository

3.1. Numerical codes and verification

The thermo-elastic solution can be obtained by solving the coupled equation of elasticity and the heat diffusion equation. The temperature calculated from the diffusion equation is transferred to the elasticity equation with an additional thermal expansion contribution from volumetric strain. Because strain energy from elasticity is insignificant compared to the effect of temperature change, the heat diffusion equation can be solved independently [2]. In order to verify the implemented thermo-mechanical calculation, two verification cases on thin and thick rectangular plates were taken from the pertinent literature, resulting in a good match between the numerical and the analytical solutions [7].

3.2. Geometry and data used for the study

No attempt was made in this study to model the geometry of the deposition holes and tunnels explicitly.

![Figure 2. Temperature evolution after emplacement of spent nuclear fuel in the repository.](image)

![Figure 3. Evolution of notable compressive stresses at selected points at a repository level of 400 m.](image)
Rather, all deposition holes and tunnels were lumped together as a thin rectangular plate of uniform thickness, and the size of the rectangle was calculated by considering the number of canisters to be disposed, the spacing of the deposition holes, and the separation of the deposition tunnels. With 6000 canisters, the spacing and the separation of the deposition holes and tunnels were 6 m and 40 m, respectively [26]. The equivalent area of the repository ($A_{rep}$) can be calculated by the following formula:

$$A_{rep} = NS_hS_c$$  \( (2) \)

where $N$ is the number of canisters, $S_h$ is the spacing of the deposition holes, and $S_c$ is the separation of the deposition tunnels. The calculated area for Forsmark was 1.44 km$^2$, and the length of the side of the whole repository was 1.2 km. Because of the symmetry of the model, the actual length of the side used in this study was 600 m. The thickness of the plate repository model was 13.3 m, based on the dimensions of the deposition holes and tunnels. The geometrical model for the reference site is shown in Fig. 1(a). In order to monitor the evolution of important variables, such as temperature and stress, monitoring points were established in four hypothetical boreholes, as indicated in Fig. 1(b). Heat-decay data from the canister were taken from the Swedish model and rock properties, in-situ stress, and initial temperature data are as shown in Tables 2 and 3 [18,27].

3.3. Temperature evolution

The maximum temperature in the rock mass was around 42°C after 100 years in the vicinity of the repository as shown in Fig. 2. At mid-depth monitoring points, which were 200 m deep, the maximum temperature was about 24°C, which was reached at about 1000 years. This different time frame for maximum temperature is an important factor when evaluating corresponding stress changes at various locations.

3.4. Thermal stress evolution

3.4.1 Evolution of thermal stresses at selected points

The thermal stress evolutions around the repository are presented in this section. Compressive, tensile, and shear thermal stresses can be generated in the present geometry of the deep geological repository at different time scales. The evolutions of stresses in the horizontal direction at various points at the repository level are shown in Fig. 3. The maximum horizontal compressive stress of 20 MPa was observed at the center of the repository after about 100 years, and it was isotropic. At the periphery of the repository, the magnitudes were smaller, with a maximum stress of approximately 10 MPa. Notable anisotropic horizontal compressive stresses (B3 and C3) were observed near the periphery of the repository. Furthermore, the time for maximum compressive stress to develop varied from 100 to 1000 years, depending on the location of the monitoring points.

It was interesting to note that significant tensile stress developed at various locations around the repository (Fig. 4). The maximum tensile stress was on the order of 10 MPa at the ground surface, directly above the center of the repository. The maximum tensile stresses were observed at the ground surface about 1000 years after deposition. Transition from tensile to compressive stress occurred at about the mid-depth point above the repository (A2 and B2). Even though tensile stresses near the
surface were in the horizontal direction, vertical tensile stresses were observed at the repository level in the vicinity of the repository (points C3 and D3). The maximum magnitude of the shear stresses was on the order of 2–3 MPa which was not negligible. It was noted that thermally-induced shear stresses at the side of the repository (B2, C2) acted in vertical planes (i.e., the xz-plane or the yz-plane, with a vertical z-axis), and shear stress at the corner (D2, D3) acted in the horizontal plane. These shear stresses will induce a rotation of the direction of the principal stress and possibly cause shear slip of the shallow dipping fractures and vertical fractures.
Transitions of the stress state with the generation of thermal stress at different locations are shown in Fig. 5. In each figure, effective stresses considering pore pressures were plotted in terms of Mohr Circles. The friction coefficients used for the upper and lower bounds were 1.0 and 0.6, respectively [28]. At location A3 at a depth of 400 m, the range of orientation that was prone to shear slip greatly increased after 100 years due to the comparatively high horizontal stress, as shown in Fig. 5(a). After 1000 years, the contribution of thermal stress to the

Figure 7. Probability of shear slip with time using general data with random distribution - (a) A3, B3, C3, and D3; (b) A2, B2, C2, and D2.

Figure 8. Probability of shear slip with time using data from Forsmark - (a) A3, B3, C3, and D3; (b) A2, B2, C2, and D2.

Figure 9. Evolution of shear slip zone with time, showing the shear slip zone (red area) and the distribution of actual fracture data from Forsmark (dotted). (a) Location A3, and (b) location B2.
shear of fracture was less significant due to the relatively homogeneous increase of thermal stress in horizontal and vertical directions (Fig. 5(a)). After 10,000 years, the stress state essentially returned to the initial state. In location A2 at a depth of 200 m, the range of orientation prone to shear slip remained the same or decreased temporarily (Fig. 5(b)). After 100 years, the horizontal stress initially decreased due to the generation of horizontal tensile stress, which reduced the possibility of fracture shear slip. After 1000 and 10,000 years, the possibilities of fracture shear slip were essentially the same. A completely different mechanism dominated the fracture shear slip mode at location A1 on the surface (Fig. 5(c)). Because of the high horizontal tensile stress, i.e., on the order of 10 MPa, fractures were prone to tensile failure after 1000 years, as shown in Fig. 5(c). It is important to note that this tensile failure was expected much later than the shear slip, which was approximately 100 years after deposition.

3.4.2 Evolution of thermal stresses along selected monitoring lines

The distribution of thermal horizontal stresses as presented in Fig. 6(a) shows that the influence area of the tensile stress at the surface was confined mainly to the area directly above the repository and maximum tensile stress occurred at around 1000 years after deposition. Modest compressive stresses were observed with coordinates larger than 600 m. A maximum tensile stress of about 10 MPa occurred at ground surface after 1000 years. Tensile stress can be observed as deep as 220 m below the surface of the ground after approximately 100 years (Fig. 6(b)). Generated horizontal stress tended to be more anisotropic at the periphery of the repository (Fig. 6(c) and (d)). Maximum compressive stress at the repository level could be as late as 1000 years in the vicinity of the repository.

4. Probabilistic fracture shear slip analysis

4.1. Evolution of the probability of shear slip at selected points

A random-distribution case of fracture orientation was chosen in order to provide a base study that was not connected to a specific site. Fig. 7 shows the variation of the probability of shear slip with time at the eight selected points. The coefficient of friction used for the probabilistic study was 0.6, which is the lower bound of typical values [28].

Fig. 7(a) shows the probability of shear slip at randomly-oriented fractures for points A3, B3, C3, and D3. As expected, the probability of shear slip increases as the thermal stress increases. The probability of shear slip at location A3 increased to about 40%, more than double the probability of initial shear slip. This increase was the result of the thermal stress creating significant differences in the horizontal and the vertical stresses. Horizontal thermal stress is substantially larger than vertical thermal stress because of the unconfined surface, and the increased difference between the two stresses causes the increase in the size of the Mohr Circle, which results in increased probability of shear slip. The probability of shear slip decreases as thermal stress decreases, i.e., when the temperature of the repository decreases. However, it is noted that this observation does not necessarily mean the recovery of the lower permeability that existed before fracture shear slip and dilation occurred. Dilated fractures are likely to be irreversible, and this aspect was investigated further by the DFN-DEM analysis, presented in the next section.

The difference between location A3 and B3 was due mainly to the fact that A3 was located in the middle of the repository, where larger thermal stress was generated. While the maximum probability of fracture slip was observed at around 100 years at both A3 and B3, a delayed maximum probability was observed at C3 between 300 and 400 years. This difference is attributed to the delayed generation of thermal stress because C3 is 200 m away from the repository.

Interestingly, the maximum probability of shear slip at C3 was greater than the probability at B3 even though the stress variation at B3 was greater than the variation at C3. An explanation for this can be based on stress differences. While the differences between both horizontal thermal stresses at B3 are small (i.e., the thermal stresses generated in both directions are essentially the same), the stress differences at C3 are larger, and the horizontal thermal stresses are generated unevenly. Also, the tensile stress of as much as 3 MPa at C3 contributed to the higher probability. Therefore, the probability of shear slip at C3 was much greater than the probability at B3. The probability of fracture slip at D3 increased by only about 10% because D3 had less thermal stress because it was about 300 m away from the repository.
corner of the repository.

Fig. 7(b) shows the probability of shear slip with randomly oriented fractures at A2, B2, C2, and D2. As expected, the overall shape of the graph is similar to the graph shown for A3, B3, and C3. The initial probability of shear slip at A2, B2, C2, and D2 was greater than the initial probability of shear slip at A3, B3, C3, and D3 because the ratio of horizontal stress to vertical stress was greater at the shallower depth. The maximum probabilities of shear slip at B2 and C2 were larger than the maximum probability of shear slip at A3. It was noted that the shape of the graph for A2 was distinctly different from that of the other graphs. When the temperature at A2 increased, tensile stress was generated, and this generation caused a decrease in the horizontal compression explaining why the probability of shear slip at A2 decreased.

The results with actual fracture orientation data from the Forsmark site are shown in Fig. 8. The shapes of the probabilities of shear slip were largely similar to the graph in Fig. 7 with random orientation. As shown in Fig. 8, the probabilities of shear slip with actual fracture orientation were less than half the probabilities with random distribution. During 10,000 years, the maximum shear slip probability was about 20% at B2 and C2. This lower probability than the case with random orientation is explained by the fact that the orientations of four fracture sets were almost vertical or horizontal, and there were fewer fractures vulnerable to shear slip in spite of increased thermal stress. However, this result must be interpreted with caution. If different sites contain fracture sets whose orientations are vulnerable to shear slip, the probability of shear slip may become even greater than with random orientation, producing a significant effect on the performance of the underground repositories. Therefore, site-specific studies must be conducted to investigate the potential for shear slip.

In order to investigate the cause of the difference in shear slip probabilities between the random orientation and the fracture orientation data from Forsmark, we plotted the actual orientation data together with the possible range of orientations that could allow for shear slip (Fig. 9). The red-shaded area is the distribution of fractures for which shear slip can occur, while the black points are the actual fracture orientations. The evolution of the size of the shaded shear slip area shows that its size reaches a maximum at 100 years, and it then returns almost to its initial state after 10,000 years. Moreover, the shape of the shear slip area at 100 years showed that increased horizontal thermal stress dominated the state of stress and that shear slip was not necessarily focused on a particular dip direction as in the initial state.

Inspection of the stereonet shown in Fig. 9 explains why there is a difference of probability for shear slip between the random orientation and the actual fracture orientation data from Forsmark. As Fig. 9 shows, the extent of overlap of the shear slip area with the actual...
orientation is small. In Forsmark, since the NE, NS, and NW fracture sets, as shown in Table 1, were almost vertical and the SH fracture set was almost a horizontal plane, the majority of the data are less vulnerable to shear slip compared with a random orientation, even with substantially greater thermal stress. A notable difference in location B2 located at 200 m depth is the slight tilting of the shaded slip zone at 100 years, which is explained by the thermally-induced rotation of principal stress at mid-depth of the repository. Fig. 10 presents the probability of shear slip with different coefficients of friction at A3, and the dependence of the probability of shear slip on the coefficient of friction is evident.

5. DFN-DEM analysis

In previous probabilistic analyses, the fracture shear slip was examined only by implicit generation, making the quantitative evaluation of permeability difficult. However, it is important to evaluate the actual change of permeability during the cycle of changing thermal stress, which was made possible through DFN-DEM analysis. To this end, numerical experiments on permeability measurements were conducted on six models of DFN using two sets of stress paths at selected locations of the repository (Fig. 11). Six DFN models with sizes of 5 m x 5 m were generated using the DFN generator in order to represent a more general behavior of the fractured rock. It was noted that the two-dimensional DFN geometry was cut in the vertical plane along the direction of the major principal stress, which is NW-SW direction, with the trend of 1451 [7,18]. The selected locations were A3 and C3 at the repository level, where reasonable probabilities of increases in shear slip and permeability were expected. Fig. 12 shows the final stress path used for the numerical experiment.

Figs. 13 and 14 show the change in permeability in six different DFNs due to changes in thermal stress. The major mechanism that led to changes in permeability in four out of six of the models (DFN-A, DFN-C, DFN-D, DFN-F) was normal deformation (closure) of fractures.
without shear slip. This observation can be explained by the lack of optimally-oriented fractures with respect to the stress orientation and poor hydraulic connectivity in these models. Vertical permeability at the repository level is insensitive to stress changes because vertical fractures are nearly closed at this magnitude of stress. However, it was noted that this observation is highly site-specific. Furthermore, all models except DFN-D and DFN-F showed anisotropic permeability throughout the entire time scale. Only two models (especially in DFN-B and, to a lesser extent in DFN-E) showed shear slip and increased permeability with a factor of up to four. One interesting observation that deserves attention is the irreversibility of the permeability for the time scale of 10,000 years. While the changes in permeability were recovered in the models for which normal closure dominated the changes, the permeability was irreversibly recovered in the two models (Figs. 13(b) and 14(b)) in which shear slip was the dominant mechanism. This result was made possible because of the elasto-perfectly-plastic fracture model adopted in this numerical study. When fractured rock was unloaded, permeability actually increased further due to contribution from the normal opening. This increase of permeability demonstrates the importance of the irreversibility of permeability once shear slip occurs.

6. Discussion

The basic mechanism of the generation of thermal stress is the expansion of the rock coupled with the constraint imposed on the rock mass; this generates horizontal compressive stress at the repository level and horizontal tensile stress at the ground surface above the repository. However, in the case of a deep
geological repository of spent nuclear fuel, more complex thermal stresses are likely because the source of heat is not uniform with respect to time, space, and geological conditions. Importantly, the use of a full-scale, three-dimensional model of the far-field will ensure that no artifacts arise when calculating the thermal stress. We thus analyzed the changes observed in thermal stress in a more systematic manner so as to judge the potential for shear slip and permeability changes.

Fig. 15 illustrates the thermally-induced, horizontal, compressive stresses, tensile stresses, and shear stresses observed around the repository. More details of the stress plots can be found in [7]. It was noted that all three modes of stresses can increase the shear slippage potential in one way or another. Importantly, shear slip occurs on different time scales. Notable mechanisms that can affect the potential for shear slip are summarized below:

- Increased horizontal compressive stress increases the possibility of shear slip because the vertical stress component remains mostly constant with time. Anisotropic horizontal compressive stress can increase the potential for shear slip at the sides of the repository.

- Horizontal tensile stress reduces total horizontal stress and can act to reduce the potential for shear slip. However, the generation of significant tensile stress, up to 10 MPa at the surface, can cause tensile failure of fractures and deformation zones. Vertical tensile stresses generated at the periphery of the repository reduce the total vertical stress, and this increases the probability that shear slip may occur.

- Thermally-induced shear stress can contribute to the rotation of principal stresses and can thus increase the potential for shear slip in shallow-dipping and near-vertical fractures.

A key issue related to shear dilation for performance assessment of a deep geological repository is whether such significant shear dilation is expected at the moderate normal stress of up to 20 MPa [27]. Barton and Choubey presented an empirical model that predicts the dilation angle under given joint compressive strength (JCS), joint roughness coefficient (JRC), and confining stress [29]. The dilation angle is calculated to be around 51, which can be large enough to cause a significant increase in permeability with a normal stress of 20 MPa, a JRC value of 6–8, and a JCS of 100 MPa. A numerical study using the discrete element method conducted by Park and Song [30] showed that the empirical equation

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**Figure 15.** Classified regions of changes in thermal stress during operation of a spent nuclear fuel repository.
by Barton and Choubey [29] actually underestimated the dilation angle, and the magnitude of shear dilation is substantial under moderate normal stress of up to 17 MPa. Furthermore, since there was an abrupt change of permeability even with a slight change of stress, a discrete element method is required to capture the elastoplastic behavior of the fracture.

Applying the full stress path of loading and unloading on fractured rock introduced in this study goes beyond the work done in [9], which considered only a generic stress ratio without considering unloading from the cooling phase. Upon unloading, the increased permeability for the DFN-B model (Figs. 13(b) and 14(b)) did not recover to its initial state and it rather increased further due to a contribution from the normal opening. This irreversible increase of permeability has an important implication in the performance assessment of a geological repository. A field observation that supports the importance of irreversible permeability increase can be found at the drift scale 8-year heating and cooling test at Yucca Mountain in the US. It showed that five out of eleven test intervals in drill holes showed irrecoverable increase in permeability, which was explained by the permanent increase in fracture aperture due to shear dilation. However, explicit modeling of each fracture was not possible in their study [11]. The current study demonstrates that shear dilation can indeed result in the irreversible permeability increase in explicit DFN modeling.

Although the geological data for this study is based on the Forsmark site in Sweden, it is noted that the conclusion drawn here is largely generic. This analysis has implications for sites that have comparatively large horizontal in-situ stresses and relatively few fractures. The difference in the elastic modulus in intact rock and rock mass was minimal at the Forsmark site, i.e., 74 GPa versus 70 GPa, and this sparsely fractured rock mass induced higher thermal stress directly proportional to the elastic modulus. The local geological model of Forsmark defined by SKB is in the size of around 12 km² and contains four fracture domains and two rock domains that show similar composition, grain size and degree of bedrock homogeneity. There are 29 deformation zones defined as a structure 1000 m or longer in size [31]. The current study modeled only one representative rock domain and one fracture domain, so additional consideration of the other domains can provide a more comprehensive analysis for the safety assessment of the repository at the Forsmark site. Furthermore, the deformation zones were not exclusively included in the current paper. Deformation zones can actually alter the stress field significantly and can also function as fluid path ways [32]. It is likely that the risk of thersoshearing can increase with higher fracture connectivity. The possible shear slip in these deformation zones is worth further investigation. Moreover, the rock stress model suggested from the Forsmark site is not conclusive because of a different interpretation of the measured in situ stress by hydraulic fracturing and overcoring method [33]. In this sense, application of a few scenarios of rock stress model will be necessary in future modeling.

7. Conclusion

In this study, thermally induced fracture shear slip, also called ‘thermoshearing,’ was examined by conducting a three-dimensional, thermo-mechanical analysis of a repository model. Stress evolutions in selected locations showed that the main mechanisms for the generation of thermal stress that are important for fracture shear slip are the following:

- comparatively high horizontal compressive thermal stress at the repository level;
- generation of vertical tensile thermal stress directly above the repository and horizontal tensile stress near the ground surface, which can induce tensile failure of fractures;
- generation of shear stress at the corners of the repository.

The implications derived from the above mechanisms are that fractures of different orientations are vulnerable to shear slip in various locations of a geological repository. The main mechanisms used in importing stress paths were the first mechanisms, which are expected to occur near the repository without the rotation of principal stress. However, further investigation of the second and third mechanism revealed that fracture openings may occur near the surface and that rotation of the principal stress may affect the shear slip of fractures.

In order to investigate the probability of shear slip, a probabilistic analysis was conducted with random orientation and actual fracture orientation data from Forsmark. Higher probability of shear slip was expected with higher differential thermal stress. When the actual fracture orientation data from Forsmark were used, the probability of shear slip was less than 20%. This low probability is explained by the fact that the orientations of four fracture sets were almost vertical or horizontal, and there was a very small area of overlap between the possible shear slip orientation and actual orientation in spite of increased thermal stress. However, if different sites contain fracture sets vulnerable to shear slip, the probability of shear slip may become greater. Therefore, site-specific studies must be conducted to investigate the potential for shear slip in the vicinity of a repository.

Stress paths obtained from the thermo-mechanical analysis were used as stress boundary conditions in order to investigate the effect of changes in stress on permeability. The DFN-DEM analysis on six DFN models at the repository level showed that, in four of the models, normal compression dominated the closure/opening of fractures, with shear dilation being the dominant factor in the other two models. In the latter two models, modest increases of permeability up to a factor of 4 were observed during the thermal loading history.

Changes in permeability caused by shear dilation persisted after the repository cooled, explained by the irreversible fracture shear deformation after shear slip. This irreversibility contrasts with the recovered changes in permeability for models in which normal fracture
closure dominates, and this deserves consideration for performance assessment of geological repositories.

Analysis was conducted on data from the Forsmark site in Sweden, and this analysis has implications for sites that have comparatively large horizontal in-situ stresses and relatively few fractures that tend to induce large thermal stress due to higher elastic modulus of rock mass.

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