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Technical Note

2015:01

Rock Mechanics - Thermal properties and thermal modelling of the rock in a repository of spent nuclear fuel at Forsmark Main Review Phase

SSM perspektiv

Bakgrund

Strålsäkerhetsmyndigheten (SSM) granskar Svensk Kärnbränslehantering AB:s (SKB) ansökningar enligt lagen (1984:3) om kärnteknisk verksamhet om uppförande, innehav och drift av ett slutförvar för använt kärnbränsle och av en inkapslingsanläggning. Som en del i granskningen ger SSM konsulter uppdrag för att inhämta information och göra expertbedömningar i avgränsade frågor. I SSM:s Technical Note-serie rapporteras resultaten från dessa konsultuppdrag.

Projektets syfte

Det övergripande syftet med projektet är att ta fram synpunkter på SKB:s säkerhetsanalys SR-Site för den långsiktiga strålsäkerheten för det planerade slutförvaret i Forsmark. SSM har genomfört en serie modelleringar om bergets respons på värme som det utbrända kärnbränslet alstrar som en funktion av tiden. Innehållet i denna rapport är en sammanställning av de viktigaste resultaten från modelleringarna som SSM låtit utföra och presenterat i sina rapporter. De sammanställda resultaten från SSM:s modelleringar jämförs med de resultat som SKB erhållit i sina modelleringar för motsvarande problem.

Författarnas sammanfattning

Som ett led i SSM:s förberedelse inför granskningen av SKB:s ansökan om tillstånd för att få bygga ett slutförvar för använt kärnbränsle i Forsmark har SSM genomfört en serie av modelleringar som relaterar till utformningen, konstruktionen och den långsiktiga säkerheten hos slutförvaret. Flera av resultaten från modelleringarna är relaterade till den termiska utvecklingen. Denna rapport redovisar utdrag från dessa oberoende modelleringsarbeten utförda för SSM:s räkning, och jämför resultaten med dem från liknande termiska modelleringar som SKB har utfört.

Under den termiska utvecklingen hos slutförvaret som funktion av tiden kommer det att ske en expansion av bergmassan i förvarsområdet. Denna expansion kommer att generera termiska spänningar som summeras med det nuvarande spänningstillståndet hos bergmassan. Det resulterande spänningstillståndet kommer att inverka på bergmassans deformation och hållfasthet och potentiellt också på grundvattenströmningen i närområdet till tunnlar, deponeringshål samt i fjärrområdet hos slutförvaret.

INSITE ("INdependent Site Investigation Tracking and Evaluation") var en oberoende expertgrupp bestående av geovetenskapliga forskare som utsågs av den tidigare myndigheten SKI och verkade under den efterföljande myndigheten SSM med syfte att nära följa och rapportera om de undersökningar som utfördes av SKB under platsundersökningarna i Forsmark. I slutskedet av INSITE-gruppens arbete upprättades en lista ("Consolidated Review Issues list", CRI) på de delar av platsundersökningarnas resultat som krävde ytterligare kompletteringar. Denna rapport lämnar en sammanfattning av de frågor om bergets termiska egenskaper samt termiska modelleringar som enligt CRI-listan behöver ytterligare arbete av SKB (t.ex. anisotropi samt diskrepans mellan mätningar av termiska egenskaper med olika metoder).

De termiska egenskaperna hos berget i förvarsområdet är av störst betydelse för dimensioneringen av paneler, tunnlar och deponeringshål. För att säkerställa den långsiktiga tätheten och den mekaniska funktionen hos bentoniten som omger kapseln har SKB föreskrivit en maximal temperatur hos bentoniten på mindre än 100°C. Det betyder att de värmealstrande kapslarna inte kan placeras för tätt intill varandra. INSITE bedömde att SKB:s stokastiska metod för att bestämma bergets och bergmassans termiska ledningsförmåga var ny, innovativ och tillämpbar.

Totalt har sex olika simuleringsprogram använts av de grupper som genomfört termiska modelleringar för SSM:s räkning. De maximala temperaturer på 42°C till 75°C som har använts för att beräkna storleken på de termiska spänningarna är lägre än den konstruktionsförutsättning som SKB upprättat för slutförvarskonceptet KBS-3. De olikheter som redovisats vad gäller den maximala temperaturen kommer sig av huruvida man har simulerat värmetillförseln som en punktvärmekälla (deponeringshål) eller som en planvärmekälla (förvaringspanel).

SSM:s modelleringsgrupper har beräknat den maximala inducerade kompressionsspänningen som påverkar deponeringshålen, utöver det nuvarande spänningstillståndet hos bergmassan, att vara inom intervallet 16-23 MPa. Storleken på inducerade spänningar mellan modelleringsgrupperna är i god överensstämmelse och fördelar sig kring medelvärdet 20 MPa. SKB har från sina 3DEC-analyser rapporterat en spänningsökning i intervallet 20-27 MPa.

Projektinformation

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SSM perspective

Background

The Swedish Radiation Safety Authority (SSM) reviews the Swedish Nuclear Fuel Company's (SKB) applications under the Act on Nuclear Activities (SFS 1984:3) for the construction and operation of a repository for spent nuclear fuel and for an encapsulation facility. As part of the review, SSM commissions consultants to carry out work in order to obtain information and provide expert opinion on specific issues. The results from the consultants' tasks are reported in SSM's Technical Note series.

Objectives of the project

The general objective of the project is to provide review comments on SKB's postclosure safety analysis, SR-Site, for the proposed repository at Forsmark. SSM has supported a series of studies related to the thermal response with time of the bedrock at Forsmark from the heat generated by the spent nuclear fuel. This report is about a collection of the main results from independent modelling presented by several groups working on behalf of SSM. The thermal modelling results by SSM are compared with the results of the modelling performed by SKB.

Summary by the authors

In preparation for the review of SKB's license application for a disposal of spent nuclear fuel, SSM has conducted a series of modelling studies related to the design, construction and long-term safety of a repository at Forsmark. Several of the presented modelling works are related to the thermal evolution of the repository with time. This report extracts the results from independent SSM reports and compares the results with the thermal modelling performed by SKB.

In the course of the thermal evolution of the repository, an expansion of the rock mass at repository level may be expected and this will superimpose additional stresses to the in situ state of stress. This may influence the rock deformability and strength and potentially also the groundwater flow in the near- and far-field of the repository.

INSITE (INdependent Site Investigation Tracking and Evaluation) was an independent expert group of geoscientists appointed by the former authority SKI, and for most of its time acting on behalf of the successor authority SSM, with the aim to closely follow and report about the site investigations carried out by SKB. At the end of the INSITE work a list of Consolidated Review Issues (CRI) was presented to summarize previous issues communicated between SKB and INSITE at the closing stage of the site investigations. This report gives a brief summary of the issue CRI-17 that deals with thermal properties of rocks and rock masses, and thermal modelling (i.e. anisotropy and mismatch between measurements of the thermal properties obtained with different methods).

Thermal properties of the rock in the repository are of importance for the design of deposition panels, tunnels and deposition holes. To ensure the long-term sealing capacity and the mechanical function of the bentonite buffer surrounding the canisters, a maximum peak temperature of the buffer of less than 100°C is prescribed by SKB's design premise. This means that canisters cannot be deposited arbitrarily close to each other. SKB's approach for thermal conductivity modelling of the rock domains by means of stochastic simulation of Thermal Rock Classes (TRC) and their thermal conductivity was considered innovative and was approved by INSITE.

Altogether six different simulation codes have been used by different SSM teams to study the thermally induced stresses in a KBS-3V repository concept. The maximum temperatures that are used to calculate the thermally induced stresses are in the range of 42°C to 75°C and are below the design requirement of <100°C. The main difference in the handling of the maximum temperature among the modelling teams is the use of point heat sources (deposition holes) or plane heat sources (repository panels) that is related to the modelling scale.

The maximum induced compressive stress increment to be added to the in situ stresses at repository level was calculated and falls within the interval 16 to 23 MPa. The magnitudes of the induced stresses across the simulation teams are in good agreement and distribute closely around the average of 20 MPa. SKB has reported a stress increment of 20 to 27 MPa derived from 3DEC analyses.

Project information

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This report was commissioned by the Swedish Radiation Safety Authority (SSM). The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of SSM.

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APPENDIX 1

1. Introduction

The last two decades have seen substantial progress in experimental and theoretical studies of the effects of coupling temperature gradients (T), hydraulic flow (H) and mechanical deformations (M) in fractured rocks. Most of the impetus behind these efforts has been the concern about the solute transport of radionuclides through a fractured rock mass containing a heat-releasing nuclear waste repository.

Already at the beginning of the studies on deep geological disposals of radioactive waste and spent nuclear fuel in the mid '80s, it became clear that the encountered technical challenges are THM-coupled and need to be studied with suitable methods and codes (Stephansson et al., 1996). This started a strong development of coupled codes that, from a few available that could handle fully coupled THM processes for fractured rocks, have today become many more that can handle THM problems and some can treat coupled chemical problems, i.e. THMC-codes. From the work conducted within the international DECOVALEX Project (DEvelopment of COupled THM models and their VALidation Against Experiments; Stephansson et al., 1996), a large number of different test cases and benchmark tests about thermomechanical problems have been conducted over more than 20 years the project has been operating. There is a general consensus that thermal simulations give a good agreement between experimental and modelling results while simulations of stresses and displacements are more problematic.

2. Motivation of the Consultants' assignment

In preparation for the review of license application for a disposal of spent nuclear fuel submitted by the Swedish Nuclear Fuel and Waste Management Co (SKB), the Swedish Radiation Safety Authority (SSM) has conducted a series of simulation studies related to the rock excavation design, construction, operation and long-term safety of a repository for spent nuclear fuel at Forsmark (Central Sweden). The studies presented in here are related to the thermal and stress evolution of the repository with time. In this report the results presented in the different studies initiated by SSM are compared with each other and in relation to SKB's results.

Each of SSM's teams has been using one or two of the following commercial codes that are able to handle coupled problems: ABAQUS, COMSOL, FRACOD2D, PFC2D, PHASE2D and UDEC. The results obtained by SSM's teams are compared to the results presented by SKB. The evaluation of the results of each of the teams could not be conducted as a strict code comparison exercise because the given boundary conditions, parameter selection and level of detail of the model geometries were not meant to be strictly the same. The commercial code 3DEC was used by SKB in most of the thermo-mechanical analyses.

Chapter 3 in this report contains a short summary about the review work on thermal properties conducted by INSITE (INdependent Site Investigation Tracking and Evaluation) for the Swedish Nuclear Power Inspectorate (SKI) and later for SSM during the time of the site investigations at the candidate sites Laxemar and Forsmark. During that time SKB developed the strategy for thermal modelling, which was new and innovative, and introduced a probabilistic approach to data collection and analysis of rock thermal properties. Minor issues brought forward by INSITE related to collection, testing and evaluation of the thermal properties and modelling are presented in this chapter.

The first part of Chapter 4 is a review of the 3DEC simulations of temperature and stress evolution in the near-field and far-field of a repository as presented by SKB in the background reports for the license application. The second part of the chapter is a presentation of the individual SSM studies, their modelling approach, input parameters, main results about maximum temperature and stress at the level of the repository and heaving of the ground surface above the repository.

Chapter 5 contains a closer presentation of the results of the different approaches and final comparison with the data presented from the 3DEC analyses by SKB.

3. Thermal properties of the rock

The heat generated by the spent nuclear fuel in the repository will increase the temperature of the waste, canister, buffer, backfill and the rock surrounding it. To ensure the long-term safety of the engineering and natural barriers, and in particular the high compacted bentonite buffer, a maximum bentonite temperature of less than 100°C is prescribed by SKB as a design requirement. To meet this requirement SKB has to determine and use data of the thermal properties from the Forsmark site in the design work. The following section presents an overview of INSITE review comments to thermal rock modelling and thermal properties of the bedrock during the site investigations at Forsmark.

3.1. An overview of INSITE's review comments to thermal properties

The INSITE Group (INdependent Site Investigation Tracking and Evaluation) was established by SKI in 2002 and consisted of an international group of geoscientists that followed SKB's site characterization work at Laxemar and Forsmark and reported to SKI and later to SSM. The final summary report (INSITE, Chapman et al., 2010) was intended to support the regulatory review of SKB's license application for a spent nuclear fuel repository. Professor O. Stephansson was a member of INSITE and had the responsibility to report about rock mechanics, rock engineering and thermal properties of rock and rock mass.

The establishment of a list of Consolidated Review Issues (CRI) was a method to summarize issues communicated between SKB and INSITE at the closing stage of the site investigations. A list of 22 CRIs remained of the original Tracking Issue List (TIL) that was used to record how issues were raised, dealt with and closed during the site investigations and for submitting issues to SKB and receiving their response (Chapman et al., 2010). The issue CRI-17 deals with thermal properties of rocks and rock masses.

SKB has been innovative in developing a stochastic simulation approach to thermal modelling. During the more than eight years period of site investigations, SKB made a continuous development of the method and also tested and validated the approach at Forsmark and in the demonstration facilities at Äspö Hard Rock Laboratory (Kristensson and Hökmark, 2007, SKB IPR-07-01). In brief the developed methodology starts by defining the scale of the modelling, and for the Forsmark Site Descriptive Model this is the size of each of the rock domains (Figure 3.1; SKB TR-08-05). Thereafter, different thermal rock classes are determined from stochastic simulations based on the lithological data recorded from drill cores and surface mapping. Based on the thermal data measured in the laboratory of the Technical Research Institute of Sweden (SP), a spatial statistical thermal conductivity model is constructed for each Thermal Rock Class (TRC) in the domain together with its statistical distribution and variogram. Then the realisations for each TRC and thermal conductivity are merged and the result is a set of synthetic realisations of thermal conductivity for each of the rock domains. For Forsmark these domains are RFM029, RFM045 and their sub-domains. The thermal domain models for conductivity, heat capacity and anisotropy are presented for different scales (1 m and 5 m). The realisations of the conductivity and in particular the tails

of the low conductivity are of utmost importance for the thermal design of the repository layout.

INSITE had the opinion and reported to SKB that the development of the stochastic method for each rock class in the domain can be applied to other problems and parameters such as diffusion, rock strength and deformability, spalling strength, grouting properties etc. SKB responded that further applications of the method were not intended. However, the variability of the rock and rock mass in the domains and sub-domains at Forsmark calls for the application of the stochastic approach and developed methodology by SKB to other problems and parameters than only thermal.

INSITE agreed in principle with SKB's strategy to record and model the thermal properties of the rocks and rock masses at different scales. INSITE also agreed with SKB's statement in the Preliminary Safety Evaluation reports (PSE) for Laxemar and Forsmark that additional laboratory measurements are needed to know better the variability of the thermal properties at different scales.



Figure 3.1. SKB's approach for thermal conductivity modelling of a rock domain with stochastic simulation of Thermal Rock Classes (TRC) and thermal conductivity λ (after SKB 2008, TR-08-05, Figure 6-6).

Before a set of realisations of thermal conductivity in a rock domain at Forsmark can be made following SKB's thermal modelling strategy (Figure 3.1), the geological model and the measured thermal conductivity data have to pass through 7 to 8 statistical calculation steps. The result can never be verified and, as honestly stated by SKB, checking that the presented realisations reproduce the spatial models is no guarantee that the thermal model is correct. However, reliable laboratory and in-situ data are needed for modelling purposes as the lower tail of the conductivity distribution has a strong impact on the calculated spacing between the canister positions in the tunnels.

INSITE believed that care should be taken when upscaling thermal properties from the laboratory core sample scale to canister deposition hole or larger scales for thermal model assessment, and the upscaled thermal properties need to be tested and confirmed for a few representative cases.

INSITE saw the need of a better knowledge about the influence of micro-cracking, causing an increased porosity in the laboratory samples, on the thermal properties and, related to that issue, about the effect of confinement due to the virgin stress state at depth can improve the thermal properties of the rock mass. SKB refers to a literature study from the '60s and claims that different laboratory testing has shown that the difference of conductivity between dry and wet samples was small and thermal cracking is only of interest for the rock-bentonite contacts in the deposition holes and rock-backfill contact in the deposition tunnels. SKB has decided not to perform any laboratory testing where variation of thermal properties with confinements is studied, although SKB could gain from knowing the influence of stress on thermal conductivity even if it might be only an increase of conductivity within the range of 1 to 5%.

SKB has not fully considered the influence of temperature on the micro-cracking, porosity, anisotropy of the different rock types at Forsmark. Therefore, SKB has an incomplete understanding of the fundamental input parameters to solve problems related to individual thermal (T), hydraulic (H), mechanical (M) problems and fully coupled THM problems. One example is the coupled THM impact of the combined effect of excavation damage zone (EDZ), stress induced rock deformation and failure (spalling), and thermal and hydraulic driven processes.

The following issues regarding thermal properties where discussed and recommended to SKI and SSM by the INSITE group during the site investigations:

- Additional number of thermal property values is needed for the rock domain RFM045,
- The possible relationship between rock density and thermal conductivity for the two main rock domains RFM029 and RFM045 at Forsmark is worth further studying,
- SKB has conducted all laboratory testing of thermal properties on wet samples. For the scenario in which rock, buffer and backfill are dry, SKB needs to know the thermal properties for dry rock,
- SKB performed a field heater test close to drill site 7 at Forsmark. The related small laboratory tests (about 10 cm³) with TPS method (Transient Plane Source) of rock samples from the test site resulted in an anisotropy factor 1.4 for the conductivity parallel versus perpendicular to the foliation. On the other hand, evaluation of the anisotropy from the field heater test gave an anisotropy factor of 1.15. Studies about the effect of anisotropy for

the design of canister spacing and the long-term safety are missing in SKB's programme,

- SKB is using old literature information about the dependence of thermal properties on pressure and temperature. An increasing rock pressure will close flaws and micro-cracks and increase conductivity, which is favourable for the design of canister spacing. An increase in rock temperature will reduce the average the conductivity with about 10% per 100°C. Laboratory testing of pressure and temperature dependence of the thermal properties of the main rock types at Forsmark is needed for the final design of the repository,
- the long-term ventilation of the transport tunnels in each of the deposition panels might increase the rock mass temperature to a point that thermal stresses due to ventilation and to the heat pulse from the waste might lead to rock failure in the transportation tunnels,
- SKB has to perform large-scale modelling of the thermal development of the repository and in particular the effects of the heating on the about 200 m thick shallow rock mass volume above the repository where tensile stresses can occur. About half the thickness of this tensile zone consists of sheeting planes and exfoliated rock with low strength and inhomogeneous rock masses,
- SKB has in cooperation with Posiva (the Finnish Expert Organisation in Nuclear Waste Management Co) tested the Finnish TERO measuring probe for in-situ determination of thermal properties in diamond drillholes (Korpisalo et al., 2013). The instrument is available for measurement in drillholes with diameter 56 and 76 mm and the measured thermal properties are estimated by using both a numerical optimisation and a simple analytical solution by means of an infinite line source model. Values of the heat conductivity from the TERO measurements are higher than the conductivity from laboratory testing (Korpisalo et al., 2013). The availability of many different laboratory methods for testing thermal properties in laboratory and in the field means that SKB has to present a detailed strategy for determining the thermal properties of the rock for the design, thermal modelling and construction of the repository.

3.2. SKB's database of thermal properties of the rock

To ensure the long-term sealing capacity and the mechanical function of the bentonite buffer surrounding the canisters, a maximum peak temperature of less than 100°C in the buffer is prescribed in SKB's design requirement (i.e. Design Premise). This means that canisters cannot be deposited arbitrarily close to each other although unnecessary long distance between the canisters means inefficient and costly use of the existing rock volume for the repository.

SKB has measured thermal conductivity in the SP laboratory with the Transient Plane Source (TPS) method. Data from testing the main rock types from Forsmark are presented in Table 3.1. The test samples have been taken from drill cores of intact rock of representative rock types. A statistical sampling procedure for choosing the samples to be tested is missing in the work by SKB. Testing has been performed at room temperature on water-saturated disc samples with a volume of about 10 cm³. The measured mean conductivity from 74 tests of the main rock type medium-grained granite to granodiorite is 3.68 W/(mK), and the maximum and

minimum values are 4.01 and 3.25 W/(mK), respectively. For the thermal dimensioning of the repository, lower thermal conductivity values have been used as reported in Hökmark et al. (2009, SKB R-09-04). Furthermore, SKB has determined the mineral composition from modal analysis of rocks and applied the known conductivity values of the co-existing minerals to determine the conductivity of the different rock types (Self Consistent Approximation method, SCA). A fair agreement with conductivities obtained with the TPS method was achieved. In addition SKB have sent rock samples to other laboratories to confirm the results of the TPS and SCA methods. However, theoretical and laboratory methods applied for determining thermal properties give different results.

3.3. Alternative methods for measuring thermal properties of the rock

In a recent paper Pasquale et al. (2015) measured rock thermal properties with a renewed version of the so-called Transient Divided Bar method (TDB). A cylindrical specimen of rock is placed between two cylindrical blocks of copper of known thermal capacity. The upper cylinder acts as a heat source and the lower more massive block as a heat sink. The heat flowing through the specimen is equal to the heat absorbed in the sink. The thermal conductivity is determined by measuring the temperature changes of the source and sink blocks. Pasquale et al. (2015) made a large number of density and conductivity tests on sedimentary and crystalline rocks.

A comparison between the results of measured heat conductivity for granite, granodiorite, tonalite and diorite obtained by SKB (Table 3.1) with those of christalline rocks obtained by Pasquale et al. (2015, Table 3.2) shows throughout higher conductivity values for the rock types from Forsmark. Despite the fact that the tested rock types are from different sites, the result of the comparison seems to indicate a systematic difference between the two methods. A comparative study of the TDB method and the commercial instrument ISOMET was done for one and the same rock sample and resulted in a conductivity difference of up to 10%. The conclusion from applying different laboratory and/or commercial systems for laboratory determination of heat conductivity is that they all give different results. The same statement is valid also for in-situ drillhole measurement results.

		Thermal conductivity k [W/(m°K)]				
Rock code	Rock name	Mean	St. dev.	Max	Min	No of samples
101057	Granitetogranodiorite, metamorphic, medium- grained	3.68	0.17	4.01	3.25	74 ¹⁾
101056	Granodiorite, metamorphic	3.04	0.09	3.20	2 .98	5
101054	Tonalite to granodiorite, metamorphic	2.73	0.19	2 .94	2.45	5
101051	Granite, granodiorite and tonalite metamorphic, fine-to medium-grained	2.85	0.26	3.39	2.46	12
101058	Granite, metamorphic, aplitic	3.85	0.13	4.06	3.68	12 ²⁾
101061	Pegmatite, pegmatitic granite	3.33	0.20	3 .50	3 07	4
102017	Amphibolite	2 .33	0.10	2.48	2.21	12
111058	Granite, fine- to medium- grained	3.47	0.17	3.62	3.22	5
103076	Felsic to intermediate volcanic rock, metamorphic	2.54		2.99	2.09	2
101033	Diorite, quartz diorite and gabbro, metamorphic	2.28				1

Table 3.1. Measured thermal conductivity λ (W/(m·K)) at room temperature (20-25°C) of different rock types using the TPS method (from SKB TR-08-05, Table 6-1).

¹⁾ Includes four oxidised samples.

²⁾ Both altered and unaltered samples included.

Table 3.2. Thermal conductivity λ and density ρ of crystalline rocks, and contents of minerals playing a major role on such parameters (Qtz - quartz, PI - plagioclase, Hbl - hornblende, OI - olivine (Fa30)). The standard deviation is shown within brackets. No is number of specimens. (After Pasquale et al., 2015.)

Lithotype	No of sampl.	Thermal conductivity k [W/(m°K)]		Density <i>ρ</i> [kg/m³]		Mineral contents (% volume)			
	No	Range	Mean	Range	Mean	Qtz	PI	Hbl	OI
Granite	22	2.44- 3.49	2.88 (0.26)	2590- 2760	2620 (20)	32	31		
Granodiorite	16	2.24- 3.03	2.52 (0.24)	2640- 2820	2690 (40)	24	44		
Tonalite	10	2.06- 2.25	2.16 (0.07)	2700- 2760	2720 (20)	19	53	7	
Syenite	3	2 19- 2.34	2.25 (0.08)	2680 - 2750	2720 (40)	4	38	18	
Diorite	14	1.73- 2.07	1.89 (0.11)	2740 - 2940	2840 (60)	5	58	23	
Gabbro	12	1.65- 2.29	1.94 (0.19)	2800- 3060	2940 (80)		53	29	3
Anorthosite	4	1.67- 1.83	1.76 (0.07)	2660- 2810	2730 (60)		80		
Hornblendite	5	2.57- 2.79	2.71 (0.08)	3020- 3180	3130 (70)			69	8
Lherzolite	11	3.31- 4.00	3.70 (0.25)	3010- 3210	3110 (50)				41
Harzburgite	3	3.52- 3.66	3.60 (0.07)	3070- 3110	3090 (20)				67
Dunite	3	4.04- 4.16	4.11 (0.06)	3320- 3360	3340 (20)				96

4. Thermal modelling of a repository of spent nuclear fuel

4.1. SKB's simulations

The strategy for thermal dimensioning of the final repository for spent nuclear fuel for the Forsmark and Laxemar sites was presented by Hökmark et al. (2009, SKB R-09-04). The strategy for dimensioning SKB's KBS-3V repository was based on the condition that the bentonite buffer temperature does not exceed 100°C for any deposited spent fuel canister. SKB used both an analytical and numerical method to determine the rock wall temperature and the peak buffer temperature. The analytical method was used to establish nomographic charts to calculate peak buffer temperature increase as a function of canister spacing for different assumption of rock conductivity (Hökmark et al., 2003, SKB TR-03-09). The developed numerical method took into account the spatial variations and autocorrelations of the thermal properties to determine the canister spacing for different rock domains at the site. The presented strategy was applied to the thermal dimensioning of Layout D2 (SKB 2009a) and in the Site Engineering Report (SKB 2009b) for the Forsmark site.

The thermal evolution of the KBS-3V repository at Forsmark and Laxemar sites has been addressed by Hökmark et al. (2010), as well as the stresses that evolve as a result of the rock expansion due to the heat. The thermal evolution is assumed to be governed by the heat emitted by the fuel and the total canister power. The thermal and thermo-mechanical properties of the surrounding rock mass were taken into account as well as the repository layout including canister and tunnel spacing. The distinct element code 3DEC was used for the rock temperature calculations. The input parameters for two of the most common rock domains are shown in Table 4.1. In situ temperatures at present day were taken from Sundberg et al. (2008, SKB R-08-65) and amount to 10.5°C at 400 m, 11.6°C at 500 m and 12.8°C at 600 m depth, respectively.

The repository layout is accurately modelled by Hökmark et al. (2010), including the distance between deposition tunnels and deposition holes. The temperature development due to the spent nuclear fuel is simulated by heat sources with an initial power of 1700 W placed at the same spacing as the deposition hole. The heat then decays with time by a power-law according to Eq. (4.1) with coefficients given in Table 4.2 (Hökmark et al., 2009):

$$P(t) = \sum a_i e^{\frac{-t}{t_i}}$$
 Eq. (4.1)

The main results from SKB's analyses are that the maximum rock wall temperature increases by about 48°C resulting in a maximum thermal stress increment of 27 MPa in horizontal direction at the repository level, for the most unfavourable deposition sequence. The canister heat decay and the resulting rock wall temperature evolution (Figure 4.1) provide the input for several of the SSM studies addressed in the next section. SKB calculated the vertical displacement of the ground surface (i.e. heave) with 3DEC by averaging it over a 400 by 400 m area directly above the repository.

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Figure 4.2 shows that the heave of the ground surface peaks with a maximum value of about 75 mm at 1000 years after the start of deposition.

Parameter	Unit	RFM029/FFM01	RFM045/FFM06
Heat capacity (C)	MJ/(m ³ K)	2.06 (2.15)	(2.12)
Mean thermal conductivity (λm)	W/(mK)	3.57	3.56
Dimensioning thermal conductivity (λd)	W/(mK)	2.9	2.55
Density (ρ)	km/m ³	2700	2700
Young's Modulus (E)	GPa	70	69
Poisson's ratio (v)	-	0.24	0.27
Heat expansion coefficient (α)	K ⁻¹	7.7x10 ⁻⁶	7.7x10 ⁻⁶

Table 4.1. Input properties for the 3DEC simulations performed in Hökmark et al. (2010).

Table 4.2. Decay coefficients for SKB reference fuel (Hökmark et al., 2009).

i-th decay coefficient in Eq. (4.1)	t _i [years]	a _i [-]
1	20	0.060147
2	50	0.705024
3	200	-0.054753
4	500	0.249767
5	2000	0.025408
6	5000	-0.009227
7	20000	0.023877



Rock wall temperature at canister mid-height

Figure 4.1. Evolution of the rock wall temperature increase at different scales for a schematic repository layout (from Hökmark et al., 2010, Figure 5-5).



Figure 4.2.Top: Heave of the ground surface after 1000 years (legend in meters). Bottom: Temporal development of the vertical displacement at the ground surface averaged over the square area marked in the upper figure (from Hökmark et al., 2010, Figure 6-17).

4.2. SSM's simulations

There are a series of SSM reports concerning the thermal evolution of the repository and the surrounding rock mass. The reports will be discussed and subsequently compared to SKB's presentation of the thermal evolution and associated stresses. The simulations performed overall yield similar results regarding the temperature evolution and also predict consistent results of thermally induced stresses and heave of the ground.

4.2.1. Shear induced fracture slip and permeability change -Implications for a long-term performance of a deep geological repository (SSM Research Report 2009:08)

This report by Min et al. (2009) is dedicated to the stress evolution due to the thermal evolution of the repository and the resulting potential for shear failure and associated increase in rock mass permeability. The simulation of stress changes due to the thermal evolution are summarised in the following.

Using a simplified geometry of the planned repository, Min et al. (2009) present a large scale simulation of the stress evolution due to the temperature changes of the surrounding rock mass in order to predict potential shear slip of fractures that can enhance fluid flow along fractures (e.g. Barton et al., 1995; Min et al., 2004). This was done using the code COMSOL Multiphysics. COMSOL is a partial differential equation solver using the finite element method (FEM).

A symmetric model geometry has been used as shown in Figure 4.3. The used material properties can be found in Table 4.3. A single heat generating plane representing the repository is assigned with a heat decay function that follows Eq. (4.1).

A time span of 10,000 years is covered in the simulation. The rock mass temperature at repository level reaches about 42°C after 100 to 500 years. The repository temperature is approaching the initial values at the end of the 10,000 years. Figure 4.4 shows the location of the monitoring points in the COMSOL model. On request by SSM, the vertical displacements and the heave of the ground surface have been extracted from the model in retrospect in 2014. The vertical displacement versus the logarithm of time for five of the monitoring points in the repository is presented in Figure 4.5. The displacement at the ground surface (monitoring point A) shows a maximum heave after 1,000 years after the start of deposition. There is a good agreement between the results of the discrete element analysis with 3DEC presented by SKB in Figure 4.2 and the finite element analysis with COMSOL in Figure 4.5.

The maximum thermally induced compressive stress increase at repository level determined by COMSOL is about 21 MPa during the thermal phase, which was modelled by means of a prescribed heat decay and related temperature evolution. These results support the findings by SKB in Hökmark et al. (2010, Section 6.2.2).



Figure 4.3. The symmetric model geometry used for the simulations with the COMSOL code (from Min et al., 2009, Figure 7).



Figure 4.4. Location of monitoring points. A1, A2 and A3 are located 200 m apart in the vertical direction (from Min et al., 2009, Figure 8).



Figure 4.5. Top: Vertical displacement at the surface at A1, B1, C1 and D1. Bottom: Vertical displacement along borehole A1. The figure is not presented in Min et al. (2009) but has been produced on behalf of SSM in 2014.

Table 4.3. Parameters used for the simulations in Min et al. (2009).

Parameter	Unit	SSM 2009:08
Heat capacity, C	MJ/(m ³ K)	2.15
Thermal conductivity, λ_m)	W/(mK)	3.58
Density, p	kg/m ³	2700
Heat expansion coefficient, α	K ⁻¹	7.7x10 ⁻⁶
initial thermal gradient	°C/m	6+0.012xz
Young's Modulus, E	GPa	70
Poisson's ratio, v	-	0.24

4.2.2. The influence of temperature and fluid pressure on the fracture network evolution around deposition holes of a KBS-3V concept at Forsmark, Sweden (SSM Research Report 2011:26)

The report presents a numerical modelling campaign on of fracture growth at small scale around deposition hole excavations using the codes FRACOD2D and PHASE2. The 2D model geometry is shown in Figure 4.6. The temperature at the bentonite-rock contact, i.e. at the deposition hole walls, is increased and decreased in steps to 15° C, 50° C, 75° C, 50° C, 25° C and 10° C, respectively. The time spans between these steps is $7 \cdot 10^8$ s (about 22.2 years) for heating and $9 \cdot 10^{10}$ s (about 2,854 years) for cooling, respectively. The employed input parameters are given in Table 4.4.

The total simulated time span for the thermal phase thus amounts to about 11,500 years. The maximum rock wall temperature is set to 75°C, resulting in a maximum thermal stress increment at repository level of about 20 MPa.



Figure 4.6. FRACOD2d model geometry for simulations performed in Backers et al. (2011, Figure 2).

Parameter	Unit	SSM 2011:26
Heat capacity (C)	MJ/(m ³ K)	2.09
Thermal conductivity (λm)	W/(mK)	3.68
Heat expansion coefficient (α)	K ⁻¹	7.7x10 ⁻⁶
Young's Modulus (E)	GPa	76
Poisson's ratio (v)	-	0.23

Table 4.4. Parameters used for the simulations in Backers et al. (2011).

The numerical analysis with FRACOD2D was mirroring the estimated stress boundary conditions for the set of input parameters presented in Table 4.4. The following steps were carried out for the analysis:

- generation of geomechanical/geometrical model and DFN fracture model,
- insertion of the excavations,
- application of swelling pressure from the high-compacted bentonite,
- application of temperature increments in the deposition holes,
- decrease of temperature in steps,
- increase of vertical stress due to ice load,
- application of water head as caused by ice load assuming hydraulic connection to the ice surface.

Figure 4.7 shows the temperature (left) and stress evolution on a horizontal plane around two deposition holes (right) for step A, F, G and K of the modelling without DFN realisations. The virgin rock temperature is assumed equal to 10.5°C and the boundary stress field is according to Martin (2007, SKB R-07-26), as shown in step A. The increase in maximum horizontal stress around the deposition hole from maximum heating of 75°C is 20 MPa (step F). After about 3,000 years the temperature at the wall of the deposition hole is reduced to 51°C and the maximum compressive stress is slightly reduced (step G). Step K shows the deposition hole with a maximum stress of 84 MPa from an assumed ice load and full hydraulic head from the top of the ice to the repository and a the temperature of ca 10°C. When simulations were done without fracture network no fractures were initiated during any step of the simulation.

When a model with realisation No I of the DFN fracture network and the high in situ stress field according to Martin (2007) is subjected to the modelling sequence with step A to K, only a few fractures propagate due to excavation and heating. The load increase due to the ice sheet gives minor propagation of the fracture network. The increase of fluid pressure from the top of the ice sheet to the repository generates fracture propagation and new fractures that may lead to potential flow paths between the deposition holes. Fracture evolution from the last step of the modelling with fracture network IM-9 and for high stress conditions is shown in Figure 4.8.

Modelling of the fracture initiation and propagation with two different stress scenarios, high stress according to Martin (2007) and low stress according to Ask et

al. (2007, SKB P-07-206), and two different fracture networks and glacial scenarios was carried out. The simulation results show that during operation, closure and thermal phase of the repository no major fracture propagation is observed that can cause hydraulic connection between the deposition holes for the high stress rock condition. A low magnitude stress field gives less confinements and frictional strength to the fractures in the DFN. Therefore, there is a potential for fracture propagation and increased hydraulic connectivity during the thermal phase. An increase of water head has the most impact on the fracture network evolution. This is illustrated in the summary diagram of the modelling results in Figure 4.9.

Step A. The excavations are introduced in the static stress field according to Martin (2007). The rock mass temperature is 10.5° C and the air temperature in the unsupported deposition holes is 14.5° C. // max. T = 14.5° C, max S1 = 79 MPa.



Step F. The temperature at the face of the deposition holes is increased to 75° C. Exposition time approx. 22 years // max. T = 75° C, max S1 = 89 MPa.



Step G. The temperature at the face of the deposition holes is decreased to 50°C. Exposition time approx. 3000 years. // max. T = 51° C, max S1 = 82 MPa.



Step K. The water head is increased by 30 MPa due to an assumed ice cover fully hydraulically connected to the repository. // T ~ 10° C, max S1 = 84 MPa.



Figure 4.7. Temperature and stress evolution of the FRACOD2D model for selected simulation steps (from Backers et al., 2011, Figure 13).



Figure 4.8. Example of the fracture evolution in a stress field according to Martin (2007) showing the last stage of the simulation with fracture network IM-9 (from Backers et al., 2011, Figure 14).



Figure 4.9. Summary of the main modelling results from Backers et al., 2011 (Figure 21). The different phases of the simulation are given along the horizontal direction, while the two assumed DFN realisations are given in the vertical direction. The top lines are for the stress field by Ask et al. (2007), the bottom lines are for the stress field by Martin (2007). The diagram shows that DFN I subjected to water head increase during glaciation is the most severe case for both stress fields. The low stress field by Ask et al. (2007) also enhances fracturing during the thermal cycle.

4.2.3. Review of Engineering Geology and Rock Engineering aspects of the construction of a KBS-3 repository at the Forsmark site – Initial Review Phase (SSM Technical Note 2012:39)

The study by Eberhardt and Diederichs (2012) generally reviews the reporting by SKB about Engineering Geology and Rock Engineering and finds that the collected geomechanical data is good in scope and quality. Nevertheless, the Authors try to

assess the impact of uncertainties of the input data on the repository design and mapping results with focus on the rejection criteria for choosing the suitable deposition holes and the capacity of the repository.

With respect to the thermal evolution and thermally induced stresses, the Authors raise the question of the effects of the variability of the encountered rock types at the site. Low conductivity rocks, such as amphibolites, tonalite, diorite dykes, may be encountered at Forsmark. It seems that lenses of amphibolite are considered in the stochastically derived distributions of thermal properties but diorite dykes, dyke swarms of smaller amphibolite lenses have not been considered by SKB. Also the effects of alteration phenomena on the thermal properties of the rock, like quartz dissolution, are not accounted for by SKB.

The main conclusion regarding thermal properties is that the associated uncertainties about quartz dissolution and precipitation should be considered because they may contribute to increase the extent of thermal spalling. It is also suggested that the exclusion of deposition holes in low thermal conductivity rock should be included by SKB in the rejection criteria for the detailed design of the repository.

4.2.4. Rock Mechanics - Confidence of SKB's models for predicting the occurrence of a damage zone around the excavations (SSM Technical Note 2013:35)

This report evaluates SKB's view on the formation of an Excavation Damaged Zone (EDZ) around the excavations in the planned repository at Forsmark (Ofoegbu and Smart, 2013). In this context, a series of simulations is performed with the commercial code ABAQUS to assess the effects of different loading scenarios using the small scale model geometry shown in Figure 4.10 with input parameters given in Table 4.5.

During the temperate phase, the governing effect is the loading due to the in situ stress around the excavation, the heat from the emplaced waste, the groundwater pressure, and the swelling pressure of buffer and backfill. The temperature evolution of the repository is taken from Hökmark et al. (2010, SKB TR-10-23) and is applied to the wall of the deposition hole, which reaches a maximum temperature of 58°C after 30 years after the start of deposition, see Figure 4.11.

The modelling results are summarised in Table 4.6, indicating for each combination of input parameters (i.e. for Model 1 to 8) if rock damage is to be expected and if so at what positions in the model. Modelling with ABAQUS indicates that the mechanical condition for the repository at Forsmark are not likely to result in rock damage if the disposal tunnels are oriented parallel to the direction of the maximum horizontal principal compressive stress (N145°E). If the tunnel axis deviate more than 45° from the direction of the maximum horizontal stress, inelastic deformation and failure will develop in the rock mass as indicated by Model 6 and 7 in Table 4.6. An uncertainty of $\pm 15^{\circ}$ of the orientation of the horizontal principal stress relative to the tunnel orientation is included in the assessment.

The maximum stress around the excavation is reported graphically in the appendix of the report by Ofoegbu and Smart (2013) and amounts to 129 MPa at the wall of the deposition hole at the peak of the thermal pulse at 37 years after deposition.



Figure 4.10. Quarter-symmetrical model geometry used in the ABAQUS simulations by Ofoegbu and Smart (2013, Figure A.2-1).

Parameter	Unit	SSM 2013:35
Heat capacity (C)	MJ/(m ³ K)	2.06
Thermal conductivity (λm)	W/(mK)	3.57
Heat expansion coefficient (α)	K ⁻¹	7.7x10 ⁻⁶
Young's Modulus (E)	GPa	70 - 78
Poisson's ratio (v)	-	0.23 - 0.24

Table 4.5. Parameters used for the simulations with ABAQUS by Ofoegbu and Smart (2013).



Figure 4.11. Temperature versus time function applied to the wall of the deposition hole during heat transfer analysis by ABAQUS calculations (from Ofoegbu and Smart, 2013, Figure A.2-2).
Table 4.6.Summary of numerical models used to evaluate the mechanical behaviour of near-
field host rock in the deposition area. The orientation of the maximum horizontal stress is
assumed to be N145°E (from Ofoegbu and Smart, 2013, Table 1).

Model	Material property set	Material property modification	Deposition tunnel orientation	Inelastic deformation (rock damage)
1	Mean intact rock	None	145°	Did not occur
2	Mean intact rock	Minimum tensile strength	145°	Did not occur
3	Mean intact rock	Maximum Young's modulus and minimum tensile strength	145°	Did not occur
4	Mean rock mass	None	145°	Did not occur
5	Mean rock mass	None	167.5°	Did not occur
6	Mean rock mass	None	190°	Tunnel floor and wall.
7	Mean rock mass	Strain-hardened tensile strength	190°	Tunnel floor and wall + deposition hole top
8 (glacial loading superimposed on stresses from case 5)	Mean rock mass	None	167.5°	Did not occur

4.2.5. Rock Mechanics – Confidence of SKB's models for predicting the occurrence of spalling (SSM Technical Note 2014:10)

Backers et al., 2014 performed simulations of the repository using the COMSOL multi-physics software package for predicting the occurrence of spalling around the excavations. The model geometry is a simplified representation of the in situ conditions at Forsmark (Figure 4.12) and the repository layout (Figure 4.13). The parameters used in the modelling are shown in Table 4.7.



Figure 4.12. COMSOL model geometry used for the simulations performed in Backers et al. (2014, Figure 4.2).



Figure 4.13. Model of the repository layout for simulation with COMSOL. Left: The repository layout is modelled as four patches of rectangular shape, for the basic simulations the model is cut into two; Right: only the lower left half with respect to the symmetry plane is used in the simulation (after Backers et al., 2014, Figure 4.6).

Parameter	Unit	2014:10
Heat capacity (C)	MJ/(m ³ K)	2.06
Thermal conductivity (λ)	W/(mK)	3.57
Heat expansion coefficient (α)	K ⁻¹	7.7x10 ⁻⁶
Young's Modulus (E)	GPa	70
Poisson's ratio (v)	-	0.24

Table 4.7. Parameters used for the simulations with COMSOL in Backers et al. (2014).

The temperature evolution is taken from the simulations in Hökmark et al. (2010). The reported rock wall temperature is assigned to the repository patches according to Figure 4.14. The resulting temperature evolution in the model is shown in Figure 4.15 for selected points in time. The thermally induced strain ε_{th} results from the relation:

$$\varepsilon_{th} = \alpha_{th} (T - T_{ref})$$
 Eq. (4.2)

where α_{th} is the thermal expansion coefficient, *T* is the temperature and T_{ref} is the strain-free reference temperature.

The total time span simulated for the thermal phase amounts to ca. 10,000 years. The initial temperature gradient with depth is 23°C/km, with a temperature of 11.5°C at repository depth. The maximum temperature of the repository patches is set to 48°C, resulting in a thermal stress increment of about 16 MPa for the horizontal principal stresses at the level of the repository (Figure 4.16). The heave of the ground surface above the repository calculated with the COMSOL model is shown in Figure 4.17 and amounts to a maximum of 14 cm after 1000 years. Backers et al. (2014) developed an alternative model for the in situ stresses at Forsmark ("geomecon model") that is believed to suit well the available in situ stress measurements and geological structures at the site.



Figure 4.14. Temperature of the repository panels versus time (from Backers et al., 2014, Figure 4.9).



Figure 4.15.Simulated temperature evolution during the heating phase in the COMSOL models. The initial temperature gradient with depth is $23^{\circ}C/km$, with $11.5^{\circ}C$ at repository depth (from Backers et al., 2014, selected time steps from Figure 4.12).



Figure 4.16. Evolution of principal stresses with time at the centre point of patch B. The background stresses are according to the geomecon model (after Backers et al., 2014, Figure 4.25).



Figure 4.17. Evolution with time of the maximum heave of the ground surface above the repository. A maximum heave of 14 cm is reached after 1000 years. This figure is not presented in Backers et al. (2014) but has been produced on behalf of SSM in 2014.

4.2.6. Relation between earthquake magnitude, fracture length and fracture shear displacement in the KBS-3 repository at Forsmark (SSM Technical Note 2014:59)

Yoon et al. (2014) address repository integrity during the phase of thermal loading and during potential seismic events at deformation zones, as well as combination of these two scenarios. All simulations are conducted with the 2D Particle Flow Code

(PFC2D). The code applies the Bounded Particle Model (BPM) where rock is assumed to behave like a cemented granular material in which both the cement and the particles are deformable and can break.

The model geometry includes deposition holes arranged in four panels named A to D, which corresponds to the layout D2 used by SKB. The deposition holes are represented by heating source particles in the models. The initial power of a canister is assumed to be 1,700 W (Hökmark et al., 2009) and the heat decay is modelled according to Eq. (4.1), resulting in 48°C maximum temperature of the heating particles (i.e. wall of the deposition holes).

Modelling of thermally induced seismicity and target fracture response due to the generated heat of the canisters disposed in the repository is carried out. The source particles emit heat to the surrounding particles through their contact points. Figure 4.18 shows the location of the canister deposition holes as point heat sources in the four panels and with two different DFN fracture network realisations.



Figure 4.18. Horizontal section models. Location of canister holes in deposition tunnels in the four panels at Forsmark for two different fracture networks, realisations (a) DFN03h and (c) DFN06h, respectively. In (b) and (d), distribution of particles that act as point heat sources in the four panels. Deformation zones are shown with green lines and DFN fractures with black lines (from Yoon et al., 2014, Figure 25).

Parameter	Unit	SSM 2014:59
Heat capacity (C)	MJ/(m ³ K)	2.06
Thermal conductivity (λ)	W/(mK)	3.57
Heat expansion coefficient (α)	K ⁻¹	7.7x10 ⁻⁶
Young's modulus (E)	GPa	70
Poisson's ratio (v)	-	0.23

Table 4.8. Parameters used for the simulations in Yoon et al. (2014).

Three different sets of in situ stresses were applied for the horizontal section model. The first set corresponds to the stress model by Martin (2007). The other stress fields simulate the conditions that might evolve at certain times (i.e. forebulge, maximum ice thickness and ice retreat) during next glaciation cycle. The mechanical and thermal properties applied are presented in Table 4.8.

Thermal evolution of the repository is modelled for simultaneous heating as well as for sequential heating where the panels are activated one by one. The timing of panel activation and the produced heat results from the number of canister positions in each panel which in turn slightly varies for each of the DFN realisations since some deposition holes are rejected by applying SKB's full perimeter intersection criterion (Munier, 2010, SKB TR-10-21).

The report refers to Min et al. (2014) for the timing of maximum thermal stresses in the near field (i.e. about 25 years after the start of deposition). Results are presented as shear displacements depending on the trace length of deformation zones and target fractures, and as a function of the distance from the active zone. Also the spatial distribution of thermally induced seismic events is shown. Intermediate results like thermally induced stresses are not reported.

4.2.7. Rock Mechanics - Evolution of fracture transmissivity within different scenarios in SR-Site (SSM Technical Note 2013:37)

The report addresses the evolution of transmissivity, including its evolution during the phase of thermal loading. Therefore, 2D simulations are performed with UDEC. The canisters therein are represented by rectangular or circular elements in the model cross sections. Those are assigned with an initial power of 1,700 W and the decay is realized by Eq. (4.1) as in Hökmark et al. (2009). The model geometry is given in Figure 4.21 and the used parameters in Table 4.9.

This results in a maximum temperature measured at the deposition hole wall of about 50° C after 25 years as shown for monitoring point B in Figure 4.22. The monitoring points from A to E in the figure are located at a distance of about 0.5 m, 0.9 m, 5.9 m, 10.4 m and 14.9 m from the centre of the heat source at a depth of 468 m.



Figure 4.21. Representation of the sections used for 2D model simulations with UDEC (from Min et al., 2014, Figure 16).

Table 4.9. Parameters used for the simulations in Min et al. (2014).

Parameter	Unit	SSM 2014:37
Heat capacity (C)	MJ/(m ³ K)	2.06
Thermal conductivity (λ)	W/(mK)	3.57
Density	kg/m ³	2700
Heat expansion coefficient (α)	K ⁻¹	7.7x10 ⁻⁶
Young's Modulus (E)	GPa	70
Poisson's ratio (v)	-	0.24
Specific heat	J/(kg°C)	762.96



Figure 4.22. UDEC modelling of the temperature variation with time for monitoring points located at different distances from the centre of a canister. The points are aligned between points A at the wall of the deposition hole, to point E about 15 m away from the canister centre on a horizontal plane (from Min et al., 2014, Figure 19b).

The initial in situ stresses plus the thermally induced stresses versus time are shown in Figure 4.23 for different monitoring points at a depth of 468 m below ground surface in Forsmark. The total induced maximum horizontal stress after heating becomes about 48 MPa, were the stress concentrations due to the presence of the deposition hole is not considered. The total induced maximum vertical stress without considering the effect of the deposition hole reaches 27 MPa and the stress ratio at the wall becomes almost 4 in the two-dimensional analysis.

The results presented in Figure 4.22 and 4.23 are valid for thermo-mechanical modelling with the assumption of homogeneous, isotropic and elastic material, see Table 4.9. UDEC analyses have been conducted for each of the NE-sections, SW-sections and horizontal sections. The mechanical properties of the rock fractures from domain FFM01 at Forsmark are presented in Table 4.10.

The temperature in the NW and horizontal sections in two-dimensional UDEC models with implemented DFN models resulted in a slightly higher maximum temperature of about 55 $^{\circ}$ C after 25 years from start of deposition.



Figure 4.23. UDEC modelling of initial in situ stress plus thermal stress in horizontal direction (a), and vertical direction (b) and stress ratio (c) versus time at five monitoring points A to E at depth of 468 m at Forsmark, without considering the stress concentrations due to the presence of the deposition holes (from Min et al., 2014, Figure 20).

Material property	Unit	Fracture (FFM01)	Comment
Shear stiffness	GPa/m	34	
Normal stiffness	GPa/m	656	
Friction angle	0	35.8	
Dilation angle	o	3.2	
Cohesion	MPa	0.5	
Tensile strength	MPa	0	
Z-dilation	m	3 x 10 ⁻³	Critical shear displacement when dilation stops
Residual aperture	m	2 x 10⁻⁵	
Zero aperture	m	3 x 10⁻⁵	

Table 4.10.Mechanical properties of the rock fractures from domain FFM01 at Forsmark used for the independent TH modelling in Min et al. (2014; after Hökmark et al., 2010).

5. Comparisons between the thermal modelling results by SKB and by SSM

The most important input parameters and main results from the thermal modelling by SKB and SSM are shown in Table 5.1.

In all SSM reports, the stresses induced by the thermal evolution of the repository are obtained by imposing the temperature. Thereby the temperature evolution is assigned to the representations of the repository plane, vertical section or single deposition hole. While some reports calculate the temperature curves from the heat decay function provided by SKB, others take the temperature increase as a function of time at the deposition hole wall as reported by SKB.

The difference in the modelling of heat sources mostly results from the different scales of the models. Thereby, it is important to note that the calculations of the thermal evolution, the associated stress field evolution or the heave of the ground surface are not the ultimate goal in none of the reports. The thermally induced stresses are an intermediate result that serves to infer potential risks to the repository integrity represented by e.g. slip on fractures, excavation damage zone, spalling around excavations, fracture transmissivity, etc. Depending on the purposes of the simulations, the model sizes also vary significantly from near-field simulations some 12 m around the deposition holes, to large-scale simulations on km-scale that include the whole repository and adjacent regional deformation zones.

It should also be noted that the comparability between the SSM reports is limited since different simulation tools have been used with each one having its own specific restrictions and requirements for input parameters. On the whole, however, there is a good agreement between the results of the different studies by SSM and the results presented by SKB.

5.1. Comparison of the input parameters for the thermal modelling

The most important input parameters for numerical simulations of the thermal evolution of the repository that have been used in the SSM reports are shown in Table 5.1. These do not differ significantly between the reports, since they are directly extracted from the SKB reports.

5.2. Comparison of the maximum rock wall temperature

The assumed maximum rock wall temperature varies throughout the reports and ranges from 42°C to 75°C, with the majority of the reports using 48°C, which is directly derived from SKB's results. There is, however, a difference in rock wall temperatures being assigned to the point heat sources (i.e. deposition holes) or to the plane heat sources (i.e. repository patches). Thereby, the two COMSOL simulations, which are far-field simulations, do not feature deposition holes but equivalent planar elements representing the repository and thus use a plane heat source. The other

reports present near-field models at the scale of several deposition holes. The PFC simulation is somewhat outstanding because it uses point heat sources for a far-field simulation, with the single heat generating particles representing each deposition hole.

In theory, if the issue was to perform a strict model comparison, the deposition holes should have been assigned the initial temperature resulting from the assumed thermal gradient plus the rock wall temperature increase of 48°C reported by Hökmark et al. (2010) in all cases. The repository patches representing the array of deposition tunnels and holes will have a lower average temperature. On the other hand, simulations that assign the rock wall temperature to the whole repository as a plane or an array of single patches will tend to overestimate the thermally induced stress increments because they neglect the rock mass between the deposition holes where there is no heat generation. SKB shows that the maximum rock temperature at repository level is on average only about 26°C (Hökmark et al., 2010, Figure 5-11).

5.3. Comparison of the maximum induced stress increments

The stresses that result from the thermal expansion of the rock mass are similar for each of the SSM reports and range between 16 and 23 MPa despite larger differences in the assumed maximum rock wall temperatures. Since the heat expansion coefficient is the same throughout all the reports, the origin of the differences could be attributed to:

- scale effects, i.e. size of the model and model elements, that differ significantly between the reported simulations,
- different thermal and thermo-mechanical properties,
- different representation of the heat sources and canister positions,
- different choice of monitoring points within the models.

The magnitudes of thermally induced stresses across the SSM reports are however in good agreement and distributed closely around the average of 20 MPa. The values reported by SKB are marginally larger and within a range between 20 and 27 MPa, depending on the monitoring location and deposition sequence of the canisters (Hökmark et al., 2010, Figure 6-6).

However, the simulations with ABAQUS presented by Ofoegbu and Smart (2013) result in a maximum thermally induced stress increment of 89 MPa. This value is much larger than results from SKB and the other SSM reviews and cannot be directly compared since this is the stress increment measured directly at the wall of the deposition hole and take into account, not only thermal effects, but also the mechanical stress concentrations due to the presence of the deposition hole itself.

5.4. Comparison of the heave of the ground surface

The evolution of horizontal compressive stresses and vertical tensile stresses as a result of the heating and expansion of the rock mass leads to a heave of the ground surface. According to SKB's simulations, the heave of the ground surface amounts to about 7.5 cm after 1,000 years (Hökmark et al., 2010).

Table 5.1. Comparison of the input parameters and main results used in different SSM reports. Alternative values are given in brackets. Z is the depth in metre.

	•	SSM 2009:08	SSM 2011:26	SSM 2013:35	SSM 2014:10	SSM 2014:59	SSM 2013:37
Authors		Min, Stephansson, 2009	Backers, Stephansson 2011	Ofoegbu, Smart, 2013	Backers, Meier, Gipper, Stephansson, 2014	Yoon, Stephansson, Min, 2014	Min, Lee, Stephansson, 2013
Simulation tool		COMSOL, UDEC	FRACOD2D, PHASE2	ABAQUS	COMSOL	PFC	UDEC
Input Parameters							
Heat capacity (C)	[MJ/(m ³ K)]	2.15	2.09	2.06	2.06	2.06	2.06
Thermal conductivity (λ)	[W/(mK)]	3.58	3.68	3.57	3.57	3.57	3.57
Density (ρ)	[kg/m ³]	2700		2700	2700	2700	2700
Young's Modulus (E)	[GPa]	70	76	70 (72)	70	70	70
Poisson's ratio (v)	[-]	0.24	0.23	0.24	0.24	0.23	0.24
Heat expansion coefficient (α)	[K ⁻¹]	7.7·10 ⁻⁶	7.7·10 ⁻⁶	7.7·10 ⁻⁶	7.7·10 ⁻⁶	7.7·10 ⁻⁶	7.7·10 ⁻⁶
Specific heat	[J/(kg°C)]	796				792.96	762.96
initial thermal gradient	[°C/m]	6+0.012z		5.88+0.0115z	0.023z		
max rock temperature	[°C]	42			48		
max rock wall temperature	[°C]		75	58		48	50
Main results							
max induced stress increment	[MPa]	21	20	89	16	not reported	23
max vertical heave of the ground surface above the repository	[cm]	10 ¹⁾			14 ¹⁾		

¹⁾ The simulation of ground heave has not been the aim of the studies, and values were not provided in the original reports. For this reason, these results need to be treated with care. SSM 2015:01 43

Results extracted from the original simulations by Min et al. (2009) and Backers et al. (2014) report heaves of the ground surface of 10 cm and 14 cm, respectively. As the models were not built for the purpose of simulating ground heave, the results have to be treated with caution. However, the results from SSM studies are of the same order of magnitude as those obtained by SKB. The time for the maximum heave is after 1,000 years in both reports and in accordance with SKB's results. This is not surprising as the heat decay function and the related shape of the temperature curve was prescribed in the SSM studies according to SKB and no additional cooling or heating effects were considered.

The maximum heave derived as post-reporting from the original simulations as reported by Backers et al. (2014) is about 14 cm after 1000 years from deposition and approximately 6.5 cm larger than the heave calculated by SKB (Hökmark et al., 2010, Figure 6-17) at the same. The temperature increase of the deposition panels in the model in the SSM report is prescribed to about 48°C. Looking at the rock temperature increase predicted by SKB (Hökmark et al., 2010, Figure 5-11), the actual maximum rock temperature increase is only about 26°C, if simultaneous deposition is assumed. This is about half the average temperature at the rock wall of the deposition holes as in the SSM report. This difference in temperature increase causes a heave twice as large on the ground surface in the model by Backers et al. (2014) compared to other SSM studies and SKB result, and can be considered to reflect a worst-case scenario.

The simulations in the SSM studies assume pure elastic conditions without considering the softer and exfoliated rock mass near the ground surface at Forsmark. These simulations are likely to overestimate the heave of the ground surface that should be reduced by the presence of the softer buffer zone at the surface (pers. comm. Ki-Bok Min, 2014).

6. The Consultants' assessment

The present report consists of two main parts: one that covers a discussion of the thermal properties with emphasis on the thermal conductivity of the rock at Forsmark, and another that covers a comparison of the results from independent simulations of the thermal evolution and associated stresses by SSM with results obtained by SKB.

The discussion of thermal properties includes a summary of the findings from the consolidated review by the INSITE Group and their recommendations to SSM. For example, there are evidences of anisotropy of the thermal conductivity at Forsmark. However, up to today, no studies by SKB address the effect of anisotropy on canister spacing and long-term safety.

Another issue is the inconsistency between the results of thermal property values determined with different methods. It is recommended that SKB should present a strategy for determining the thermal properties for the design, construction and thermal modelling of the repository of spent nuclear fuel.

In the light of more recent publications, it has been shown that the rock thermal conductivity is not trivial to determine and the available measurement methods yield systematically different results. Since the thermal conductivity is an important parameter for the modelling of the operational and long-term safety of the repository, but also for the layout dimensioning of e.g. canister spacing and deposition tunnel spacing, there might be a need for additional modelling of the thermal phase with application of low thermal conductivities of the rock.

Results from independent modelling conducted by SSM on the issue of stress evolution around the planned repository for spent nuclear fuel at Forsmark are summarised and compared in this report. In total, six different simulation tools were used in addition to that employed by SKB. The main findings are:

- the input parameters are in agreement between the studies although the modelling approaches are different,
- the maximum stress increase reported by SKB is 27 MPa for the worst-case scenario. With exception of one of SSM's reports, the span of the maximum stress increase is 16 to 23 MPa with an average of 20 MPa.

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Coverage of SKB reports

Table A1.1: SKB reports considered in the present summary report.

Reviewed report	Reviewed sections	Comments
SKB P-07-206, Ask et al., 2007	Only reference to	Rock stress model (low stresses)
SKB TR-03-09, Hökmark and Fälth, 2003	Relevant sections	Thermal modelling strategy
SKB R-09-04, Hökmark et al., 2009	Relevant sections	Strategy for thermal dimensioning of the repository
SKB TR-10-23, Hökmark et al., 2010	Relevant sections	Thermo-mechanical modelling of the repository
SKB IPR-07-01, Kristensson and Hökmark, 2007	Relevant sections	Prototype Repository experiment
SKB R-07-26, Martin, 2007	Only reference to	Rock stress model (high stresses)
SKB TR-10-21, Munier R., 2010	Only reference to	Extended full perimeter intersection criteria
SKB TR-08-05, 2008	General	Site description of Forsmark
SKB R-08-116, 2009a	General	Layout D2 for Forsmark
SKB R-08-83, 2009b	General	Site Engineering Report for Forsmark
Sundberg et al., 2008	Relevant sections	Thermal properties at Forsmark

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