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Thermal properties at Äspö HRL

Analysis of distribution and scale factors

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Summary

A thermal model for the Äspö HRL as well as a general strategy for thermal modelling is under development. As a part of that work, thermal conductivities have been modelled from reference values of thermal conductivity of different minerals and from the mineral composition of all Äspö samples in the Sicada database. The produced thermal conductivity database has been analysed in terms of frequency, type of distribution, spatial distribution, variogram etc. A correction factor has been estimated to compensate for discrepancies between measured and calculated values. The calculated values have been corrected according to measured values.

The data has been analysed according to different rock types. However, there are uncertainties in the base material of rock classification, mainly due to problem to distinguish between Äspö diorite and Ävrö granite, but also because of different classification systems.

There is a relationship between thermal conductivity and density for the rock types at Äspö. Equations of the relationship have been developed based on all thermal conductivity, heat capacity and density measurements. The equations have been tested on two bore holes at Äspö with promising results. It may be possible to evaluate the spatial distribution of the thermal properties from density loggings. However, more work is needed to develop a complete model including the handling of high and low density zones.

There is an insufficient knowledge in the variation of thermal properties at different scales. If the whole variation within a rock type is in the cm-m scale the thermal influence on the canister is small. This is due to the fact that the small-scale variation in thermal properties is mainly averaged out in the 5–10 m scale. If the main variation within rock types is in the 5–10 m scale there is probably a significant effect on the canister temperature. However, it is likely that the observed variation occurs in both these scales.

Simulation has been performed of the sensitivity in canister temperature for variations in thermal properties within one rock type and between different rock types. The results show that the canister temperature is quite sensitive to the thermal conductivity within an area, $6 \cdot 40$ m^2, around the canister. The influence is obviously largest closest to the canister. With well defined thermal properties in the tunnel area there is still a large influence on the canister temperature if low conductive rock is present outside the tunnel.

Sammanfattning

En strategi för utveckling av platsbeskrivande modell tillsammans med en termisk modell för Äspö HRL är under utveckling. Som en del av detta arbete har värmekonduktivitet beräknats från referensvärden för konduktivitet för olika mineral samt mineralsammansättningen för alla Äspö prover i databasen SICADA. Den därvid framtagna databasen över värmekonduktiviteter har analyserats med avseende på frekvensfördelning, fördelningstyp, rumslig fördelning, variogram etc. En korrektionsfaktor har tagits fram för att kompensera för skillnader mellan beräknade och uppmätta värden. De beräknade värdena har blivit korrigerade gentemot uppmätta värden.

Data har analyserats med avseende på olika bergarter. Osäkerheter förekommer emellertid i bergartsklassificeringen, huvudsakligen beroende på problem, att skilja på Äspö diorit och Ävrö granit.

Samband finns mellan densitet och värmekonduktivitet för flertalet bergarter vid Äspö. Ekvationer som beskriver sambandet ha utvecklats baserat på alla utförda mätningar av värmekonduktivitet, värmekapacitet och densitet. Ekvationerna har testats på två densitetsloggade borrhål vid Äspö med lovande resultat. Det kan vara möjligt att utvärdera den rumsliga fördelningen av termiska egenskaper från sådana mätningar. Ytterliggare arbetet krävs emellertid för att utveckla en komplett modell som även inkluderar hantering av låg- och högdensitets zoner.

Kunskapen är otillräcklig avseende variationen av termiska egenskaper i olika skalor. Om hela variationen för en bergart förekommer i cm-m skalan så är den huvudsakligen utjämnad i 5–10 m skalan och temperaturinverkan på kapseln blir liten. Om den huvudsakliga variationen förekommer i 5–10 m skalan så är den temperaturpåverkan på kapsel troligen signifikant. Det är emellertid troligt att den observerade variationen förekommer i båda dessa skalor.

Simuleringar av kapseltemperatur har utförts för variationer av termiska egenskaper för en bergart och mellan två bergarter. Resultaten visar att kapseltemperaturen är ganska känslig för förändringar av de termiska egenskaperna i den simulerade arealen runt kapsel ($6 \cdot 40$ m^2). Känsligheten är givetvis störst för området närmast kapseln men med väl definierade egenskaper in tunnelområdet så är det fortfarande en stor påverkan om avvikande egenskaper finns utanför tunnelområdet.

Contents

1 Introduction and objectives

The Swedish Nuclear Fuel and Waste Management Co (SKB) is responsible for the handling and final disposal of the nuclear waste produced in Sweden. The temperature field in the repository depends on the thermal properties of the rock and the generated heat of the deposited canisters, due to radioactive decay. The layout of the repository is dependent on the predicted temperature field. The design criterion is specified as the maximum temperature allowed on the surface of the canisters /Andersson et al, 2000/. A low thermal conductivity leads to a larger distance between canisters than in the case of a high thermal conductivity.

A series of site investigations are planned for the siting of a deep repository. For each of the studied sites design work will be carried out as a foundation for studies of constructability, design, environmental impact assessment and safety assessment. The technique for long-term storage of spent nuclear fuel is developed at the Äspö Hard Rock Laboratory.

The measured data is interpreted in terms of a site descriptive model covering geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties and surface ecosystems, in an integrated fashion.

The present report is part of the work of developing a 3D model for the thermal properties at Äspö HRL but it also supplies input to the general strategy for site descriptive modelling of thermal properties.

The objective is to perform a statistical description of the thermal properties of different rock types at Äspö HRL from the existing data. Another objective is to get a better understanding of thermal scale effects by numerical simulations based on existing data.

2 Different sources for thermal properties

The thermal properties at Äspö HRL have been studied in a number of investigations. /Sundberg, 1991; Sundberg and Gabrielson, 1999; Sundberg, 2002/. The thermal properties have been measured and compared with theoretically calculated values based on the mineral composition. Thermal measurements have been performed on 22 samples. This is a very limited database in order to describe and analyse the thermal properties at Äspö HRL.

However, other sources for determination of the thermal properties exist. A rather great number of mineral analyses exist in the Sicada database at Äspö HRL that can be used for calculation thermal properties. Further, /Sundberg, 2002/ has showed that for diorites and granites at Äspö there exists a relation between density and thermal conductivity. This implies that it is possible to use existing results from density logging in boreholes to analyse the thermal conductivity variations.

Thus, three different methods have been used to analyse the thermal properties:

- Direct measurements
- Calculations from mineral composition
- Calculations from density logging

A fourth method whereby changes in the thermal conductivity of the rock can be studied is to analyse temperature loggings in deep boreholes. Assuming a constant heat flow, a change in thermal conductivity would under ideal conditions influence the temperature gradient in the rock mass. A short study on this subject has earlier been performed at Äspö. The method is interesting but is not further discussed in the present study.

3 Measurements of thermal properties

3.1 Introduction

The thermal properties at Äspö HRL have been studied by /Sundberg, 1991/, /Sundberg and Gabrielsson, 1999/ and /Sundberg, 2002/. Measurements have been performed in the two latter investigations. These samples originate from two locations at Äspö HRL, the prototype repository and borehole KA2599G01.

Measurements of thermal properties in the laboratory were performed using the TPS (transient plane source) method /Gustafsson, 1991/. The method may be used for simultaneous measurements of thermal diffusivity and thermal conductivity of both fluids and solids and it is also recommended for the site investigations /SKB, 2001/.

3.2 Measured values

In Table 3-1 the results from all measurements are summarized. In Table 3-2, Table 3-3 and Table 3-4 the results are divided into different rock types.

Table 3-1. Results from all TPS measurements. Investigation A: /Sundberg and Gabrielsson, 1999/, investigation B: /Sundberg, 2002/.

Sample	Density (kg/m^3)	Thermal Conductivity (W/m·K)	Volumetric heat capacity (MJ/m^3·K)	Rock type	Investi-gation
KA3539-1 1.0–1.22	2769	2.42	2.22	Äspö diorite	A
KA3539-2 5.50–5.68	2716	2.63	2.14	Alt. Äspö diorite[1]	A
KA3545 0.83–1.11	2733	2.72	2.27	Alt. Äspö diorite[1]	A
KA3551 0.95–1.15	2724	2.76	2.15	Alt. Äspö diorite[1]	A
KA3563 0.88–1.12	2745	2.39	2.15	Äspö diorite	A
KA3569 0.87–1.20	2745	2.42	2.19	Äspö diorite	A
KA3575 1.03–1.27	2764	2.44	2.18	Äspö diorite	A
KA3581 1.10–1.33	2770	2.50	2.32	Äspö diorite	A
KA3587 0.97–1.14	2777	2.33	2.29	Äspö diorite	A
KA3593-1 1.42–1.63	2742	2.55	2.10	Äspö diorite	A
KA3593-2 4.19–4.43	2820	2.38	2.33	Xenolite	A
KA2599 G01 5.90–5.94	2765	2.49	2.16	Äspö diorite	B
KA2599 G01 14.63–14.67	2770	2.34	2.13	Äspö diorite	B
KA2599 G01 25.32–25.36	2755	2.47	2.09	Äspö diorite	B
KA2599 G01 44.28–44.32	2673	2.99	2.06	Ävrö granite	B
KA2599 G01 50.10–50.14	2636	3.58	1.93	Fine-gr. granite	B
KA2599 G01 61.89–61.93	2648	3.68	2.02	Fine-gr. granite	B
KA2599 G01 70.60–70.64	2708	2.84	2.10	Äspö diorite	B
KA2599 G01 85.10–85.50	2720	2.69	1.96	Äspö diorite	B
KA2599 G01 101.85–101.89	2726	3.11	2.30	Alt. Äspö diorite[1]	B
KA2599 G01 120.05–120.09	2655	3.22	1.99	Ävrö granite	B
KA2599 G01 126.35–126.39	2662	3.55	2.34	Ävrö granite	B
Mean value		2.75	2.16		
Median value		2.59	2.15		
Standard deviation		0.43	0.12		
Skewness		1.12	–0.12		

[1] Altered Äspö diorite means in this case that the biothite is replaced by chlorite.

Table 3-2. Mean values of measured thermal conductivity (W/(m·K)) (TPS method) of different rock types from the Äspö area, from different studies (Modified from /Sundberg, 2002/).

Rock type	/Sundberg and Gabrielsson, 1999/		/Sundberg, 2002/		Total	
	Number of samples	Measured, TPS	Number of samples	Measured, TPS	Number of samples	Measured, TPS
(Fresh) Äspö diorite	7	2.41	5	2.56	12	2.47
Altered Äspö diorite	3	2.70	1	3.11	4	2.80
Ävrö granite			3	3.24	3	3.24
Fine-grained granite			2	3.63	2	3.63

Table 3-3. Statistics for measured thermal conductivity (W/(m·K)) of different rock types.

Rock type	Number of samples	Mean value	Median value	Standard deviation	Skewness
Fine grained granite	2	3.63	3.63	0.07	–
Ävrö granite	3	3.25	3.22	0.28	0.53
Altered Äspö diorite	4	2.81	2.74	0.21	1.60
Äspö diorite I	12	2.49	2.46	0.15	1.44
Äspö diorite II (including altered Äspö diorite)	16	2.57	2.50	0.21	1.21

Table 3-4. Statistics for measured heat capacity (MJ/(m^3·K)) and density (kg/m^3) of different rock types.

Rock type	Number of samples	Mean value	Median value	Standard deviation	Skew-ness	Density
Fine grained granite	2	1.98	1.98	0.06	–	2642
Ävrö granite	3	2.13	2.06	0.19	0.53	2663
Altered Äspö diorite	4	2.22	2.21	0.08	0.10	2725
Äspö diorite I	12	2.16	2.16	0.10	–0.19	2753
Äspö diorite II (Altered Äspö diorite and Äspö diorite)	16	2.17	2.16	0.09	–0.27	2733

In the tables above the volumetric heat capacity (C) (MJ/(m^3·K)) is calculated from measurements of thermal conductivity (λ) and thermal diffusivity (κ) using the relationship $\kappa = \lambda/C$. Especially the thermal conductivity has strong correlation to rock type since the standard deviation is reduced, compare the standard deviation in Table 3-1 and in Table 3-3.

4 Calculations of thermal properties from mineral analyses

4.1 Introduction

Calculations of the thermal conductivity of rock can be made using reference values of thermal conductivity of different minerals and the respective volume fractions /Horai and Baldridge, 1972; Sundberg, 1988/. Different numerical solutions have been used by different authors for the calculation of thermal conductivity of soil and rock. /Sundberg, 1988/ applied a numerical solution based on the self-consistent approximation (SCA) which produced results in good agreement with measured values.

However, the self-consistent approximation uses a rather complicated iterative process for the calculation. A more simple expression is the geometric mean equation. The expression is related to the self-consistent approximation in two dimensions if the frequency function is log normally distributed /Dagan, 1979/. The geometric mean equation gives a slightly lower value of the thermal conductivity compared to the self-consistent approximation. In the present study the geometric mean equation has been used for calculation of thermal conductivity from mineral analyses in the Sicada database. This is further discussed in section 4.3.1.

The results of the geometric mean equation and the SCA have earlier been compared with measured values for the same samples. If the measured values are assumed to be "true" the calculated values can be corrected with respect to the obtained discrepancy. This correction can also be used on calculated values from the Sicada database. However, in the tables below the values are uncorrected if not the table text says otherwise.

4.2 Rock types in the Äspö area

Three main rock types have been distinguished in the Äspö area:

- Småland granitoids (Äspö diorite – Ävrö granite)
- Fine grained granite
- Greenstone

The first group, Småland granitoids, is the main rock type in the Äspö area and contains both Ävrö granite and Äspö diorite. It consists of a number of subtypes with variations in the chemical composition due to mixing and mingling processes. The transitions are often continuous and the different subtypes can not easily be distinguished by eye. However, in earlier performed rock mapping the name Smålands granite has mainly been used synonymously with Ävrö granite.

Fine-grained granite has a more acid composition compared to Småland granitoids. Both fine-grained granites and greenstones appear mainly as smaller bodies, xenolites and lenses.

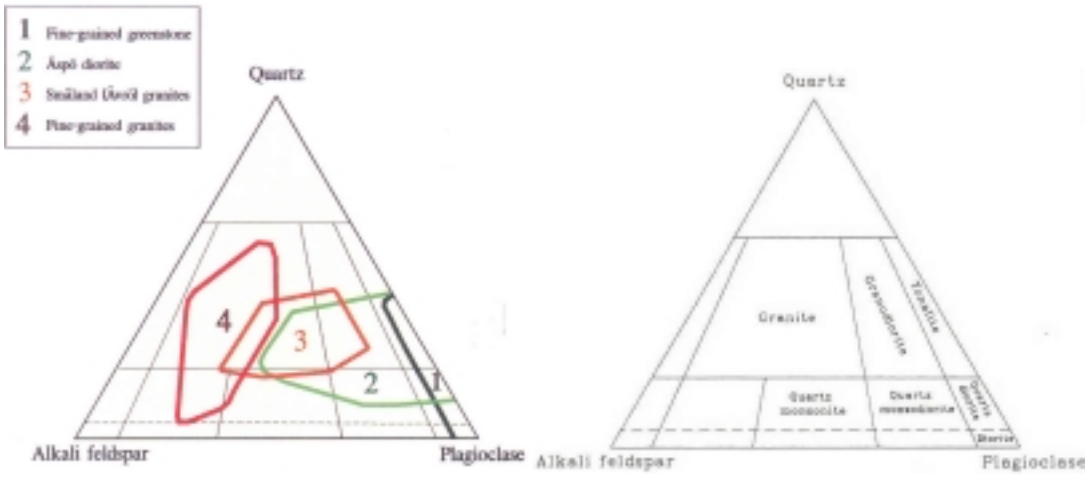

Figure 4-1. *Graph over main mineral composition of dominating rock types at Äspö /Rhén et al, 1997/.*

Another way to classify the rock samples is strictly from the mineral content. This demands modal analyses (point counting of minerals in microscope) and chemical analyses. This is the concept that has been used in Sicada and the samples have been divided in the following rock types; granite, granodiorite, quartz diorite, quartz monzodiorite, tonalite, greenstone etc. In Sicada a connection to the ocular core mapping only exists for boreholes and not for the surface mapping in the tunnel or on the ground surface.

Consequently, it is not possible to analyse the whole database on the above mentioned rock types in the Äspö area; Småland granitoids, Fine grained granite and Greenstone. However, for samples from core drilling (bore hole) it is possible to integrate data from core mapping.

4.3 Calculation of thermal conductivity

4.3.1 Method for determination of thermal conductivity

As described above, the calculations of the thermal conductivity from the mineral fractions have been made using the geometric mean equation.

The thermal conductivity is calculated from the percentage of the different minerals together with literature values of the thermal conductivity for different minerals. The geometric mean equation has the advantage of being simple to use but underestimates the calculated thermal conductivity with about 2–5% compared to the above mentioned self consistent approximation (in the conductivity interval 2.5–3.5 W/(m·K) with the lower percentage for the lower conductivity). On the other hand, the sum of minerals is overestimated with about 1.4% as a mean value. This results in an overestimation of the thermal conductivity. The total effect should therefore be in fairly good agreement with the self-consistent approximation, especially for low conductivities.

The SICADA database contains data from the whole Äspö-Simpevarp area. A special interest is connected to the area close to the Äspö HRL. This limited part of the database has therefore been studied separately. The limited data volume (LDV), a cube with the size 400·600·700 m^3, contains about half of the samples in the database, see Table 4-1.

The co-ordinates for the LDV are depth: 200–600 m, Easting: 1551100–1551700, Northing: 6367500–6368200. (Coordinate system: RT 90, RHB 70, 2.5 Gon W).

4.3.2 The SICADA database

Introduction

All data from investigations at the Äspö Hard Rock Laboratory are stored in the database SICADA. The mineral content in different rock types has been examined during different stages in the building of Äspö HRL. The samples can be divided according to the following:

- Surface samples at ground level – the initial sampling
- Samples from core drillings
- Samples from the construction of tunnel

The database on mineral analyses constitutes of the following types of parameters: ID, Rock type, Type of sampling (surface, tunnel or drill core), Positioning data and Percentage of 26 different minerals. The rock type is determined from the mineral analysis and the connection to the original ocular rock mapping is only possible for samples from boreholes.

A total of 223 mineralogical samples have been collected in the database. The sum of the mineral is as a mean greater than 100%. This is caused by errors in calculation or data input and by the fact that some minerals is detected as 0.5% when the content in reality is <0.5%. Samples have been excluded from the calculations if the sum of the minerals exceeds 103.5% or fall below 98.5%. This still results in a total mean value greater than 100% (101.4%). After these exclusions 198 samples are remaining in the database.

Rock types from mineral analyses

The samples are divided into different samplings and rock types according to Table 4-1. The diorite group consists of all samples that are not of the rock types granite or greenstone. This simplification has been done due to few samples in each sub type. Some samples has not been classified.

Table 4-1. Number of samples analysed, divided in rock type and type of sample.

Data volume /Rock type	Total	Type of sample		
		Surface	Borehole	Tunnel
All samples				
All rock types	198	33	85	80
Granite	84			
Diorite	81			
Greenstone	27			
Limited data volume				
All rock types	89	–	45	44
Granite	42			
Diorite	26			
Greenstone	13			

Rock types from core mapping

For a part of the database it is possible to group the data regarding rock types from original mapping (samples from bore holes). This makes it possible to group the borehole samples in Småland granite, Äspö diorite, fine-grained granite and greenstone. The names Småland granite and Äspö diorite may have been used for both Äspö diorite and Ävrö granite. The number of samples divided in to different rock types and data volumes is shown in Table 4-2.

Table 4-2. Number of samples analysed from boreholes, divided in rock type based on core mapping.

Rock type	Number
All samples	
All rock types	85
Ävrö granite	25
Äspö diorite	37
Fine-grained granite	10
Greenstone	11
Limited data volume	
All rock types	46
Ävrö granite	5
Äspö diorite	27
Fine-grained granite	3
Greenstone	7

4.4 Analysis of database

4.4.1 Thermal conductivity of rock types from mineral analyses

The database has been described and analysed by different tools:

- Mean, standard deviation and median values
- Histograms
- Lognormal diagrams
- Spatial sample location
- Variograms in 2 and 3 dimensions

The different diagrams are shown in Appendix 1. Note that the scale is different in the different figures.

Histogram

The histograms are more or less asymmetrical for all types of rock, see Appendix 1. The distribution of diorite samples has the most symmetrical shape. According to Table 4-3 the mean and median values are closer to each other for the limited data volume, which indicates a more symmetrical distribution.

Comparing the histograms of samples collected on surface, from drill cores and from tunnel, a difference in the distribution appears, see Appendix 1. This is also reflected in Table 4-4. The reason can be real differences in the rock composition or differences due to selective sampling.

Table 4-3. Calculated thermal conductivity, sorted by rock type (TrMean: Trimmed mean – highest and lowest 5% is excluded).

Data volume /Rock type	N	Mean	Median	TrMean	StDev	Min	Max	Q1	Q3
All samples									
All rock types	198	2.81	2.67	2.78	0.51	1.91	6.63	2.44	3.17
Diorite	81	2.50	2.46	2.49	0.22	1.91	3.14	2.35	2.66
Granite	84	3.06	3.14	3.07	0.37	2.34	3.69	2.74	3.38
Greenstone	27	2.82	2.62	2.80	0.48	2.32	3.88	2.50	2.96
Limited data volume									
All rock types	89	2.83	2.66	2.78	0.60	1.91	6.63	2.44	3.16
Diorite	42	2.48	2.46	2.47	0.22	1.91	3.09	2.36	2.57
Granite	26	3.16	3.18	3.16	0.27	2.61	3.64	2.97	3.34
Greenstone	13	2.98	2.91	2.96	0.51	2.43	3.85	2.60	3.46

Table 4-4. Calculated thermal conductivity, sorted by type of sampling (TrMean: Trimmed mean – highest and lowest 5% is excluded).

Data volume /Type of sample	N	Mean	Median	TrMean	StDev	Min	Max	Q1	Q3
All samples									
Drillhole	85	2.71	2.58	2.69	0.43	1.91	3.85	2.41	2.95
Tunnel	80	2.91	2.77	2.86	0.58	2.28	6.63	2.54	3.21
Surface	33	2.85	2.64	2.83	0.47	2.32	3.88	2.44	3.36
Limited data volume									
Drillhole	45	2.63	2.46	2.60	0.44	1.91	3.85	2.36	2.73
Tunnel	44	3.04	2.94	2.96	0.67	2.37	6.63	2.59	3.30

Test of log normal distribution

Many variables in the nature are log normally distributed. This has also been tested for the actual rock type distributions. The result is shown in Appendix 1. The diorite and granite (LDV) distributions are closest to a log normal distribution.

Geometrical distribution

The geometrical distribution of the samples has been plotted and is shown in Appendix 1. The figures show that the distribution of samples is heterogeneous but a pattern can be seen. It is actually possible to distinguish samples taken from boreholes and tunnel.

Variogram

In a variogram the variance is plotted versus lag length. The lag is the distance between sample pairs. To get one point in the diagram the variance in thermal conductivity is calculated for a certain distance (lag) between the samples (± x m interval).

Two- and three-dimensional variograms are presented in Appendix 1. The 2D-diagram is made and analysed by the data programme Surfer /Surfer, 2002/. 1D diagram along boreholes has not been made due to few data points.

It is reasonable to assume that the difference in conductivity between samples is increasing if the distance between the samples is increasing. In a variogram this is illustrated as an increasing variance with lag length. If the graph flattens at a certain variance (sill) it represents the correlation length.

A variogram also gives opportunity to study anisotropy behaviour in the thermal conductivity for the rock mass. However, in the present study few samples and uneven distribution of samples implies that analysis of anisotropy is not meaningful.

Most of the variograms in Appendix 1 can not be evaluated, probably due to the small amount of samples. For the diorite and granite there is a tendency to the curve to flatten at a lag length of about 200 m. This indicates a correlation length of about 200 m. However, due to lack of data it is not possible to make a closer investigation and examine the possibility of a more short ranged correlation length.

4.4.2 Thermal conductivity of rock types from core mapping

For samples from core drilling (bore hole) it is possible to integrate rock type from core mapping. In Table 4-5 statistics is showed for logged rock types and also the combination of Smålands granite and Äspö diorite.

Table 4-5. Calculated thermal conductivity, sorted by rock type from core mapping in boreholes (Skewness: Indicates if the distribution around the mean value is positive or negative skew).

Data volume /Rock type	N	Mean	Median	StDev	Min	Max	Skewness
All samples	**85**	**2.71**	**2.58**	**0.43**	**1.91**	**3.85**	**0.88**
Smålands granite	25	2.82	2.73	0.32	2.10	3.44	0.23
Äspö diorite	37	2.39	2.40	0.16	1.91	2.72	–0.33
Smålands granite and Äspö diorite	62	2.56	2.49	0.32	1.91	3.44	0.95
Fine grained granite	10	3.33	3.38	0.21	3.04	3.69	0.14
Greenstone	11	2.91	2.69	0.41	2.42	3.85	1.16
Limited data volume	**45**	**2.63**	**2.46**	**0.44**	**1.91**	**3.85**	**1.39**
Smålands granite	5	2.91	2.73	0.38	2.52	3.33	0.42
Äspö diorite	29	2.39	2.42	0.17	1.91	2.72	–0.45
Smålands granite and Äspö diorite	34	2.47	2.43	0.28	1.91	3.33	1.50
Fine grained granite	3	3.33	3.12	0.42	3.04	3.81	1.67
Greenstone	7	3.11	2.94	0.53	2.43	3.85	0.48

4.5 Comparison between calculated values and laboratory measurements

A comparison between measured thermal conductivity and calculated conductivity using the SCA method has earlier been made for the Äspö HRL. In the calculations above, the geometrical mean equation was used, see discussion in 4.1. In Table 4-6 measured values with the TPS-method are compared to both SCA and geometric mean equations.

If the measured values are assumed to be correct, the geometric mean equation underestimates the thermal conductivity with 9–10% depending on rock type.

Table 4-6. Comparison between laboratory measurements (TPS method) and calculated values for different rock types (SCA = self-consistent approximation, GM=Geometric mean).

Method	Äspö diorite[1]	Äspö diorite[2]	Ävrö granite	Fine-grained granite
	λ, W/(m·K)	λ, W/(m·K)	λ, W/(m·K)	λ, W/(m·K)
Calculated (SCA)	2.24	2.35	3.01	3.45
Measured (TPS)	2.41	2.56	3.24	3.63
Diff, % (SCA-TPS)/TPS	–7.1%	–8.2%	–7.1%	–5.0%
Calculated (GM)	2.19	2.33	2.91	3.30
Diff, % (GM-TPS)/TPS	–9.1%	–9.0%	–10.2%	–9.1%

[1] /Sundberg and Gabrielsson, 1999/
[2] /Sundberg, 2002/

5 Calculations of thermal properties from density logging

5.1 Equations for thermal properties

A relationship between density and thermal conductivity was found by /Sundberg, 2002/, concerning borehole KA2599G01 at Äspö HRL. Based on this investigation, a relationship between density and thermal conductivity and volumetric heat capacity respectively were derived by /Staub et al, 2003/.

However, /Sundberg and Gabrielsson, 1999/ also presented results from laboratory measurements on thermal properties at the prototype repository at Äspö HRL. When data from both these investigations /Sundberg, 2002; Sundberg and Gabrielsson, 1999/ are used (in total 21 samples), new relationships are derived and shown in Figure 5-1.

Four of the samples consist of altered Äspö diorite, which have biotite replaced by chlorite. Equations are derived both when these values are included and when they are excluded, see Equation 5-1 to 5-4. The fit (R^2) of the regression line to the data is in general better if the altered samples are excluded.

One of the samples from the earlier investigation consisted of xenolith (basic volcanite). Values from this sample are excluded from the calculations.

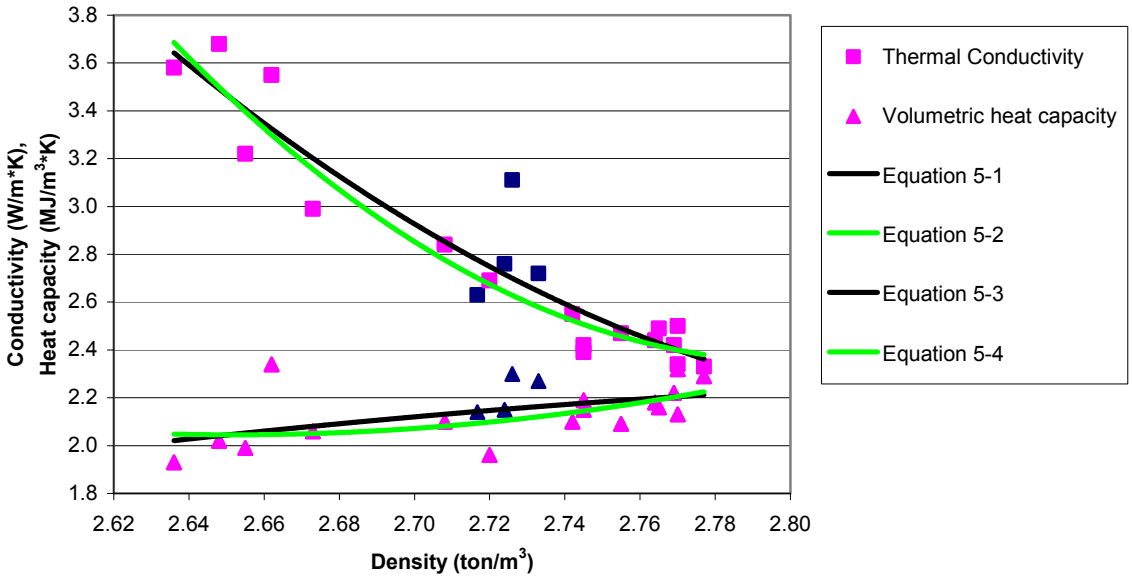

Figure 5-1. *Relationships between density and thermal properties. Values from altered Äspö diorite are marked with dark blue colour. Equations are derived by polynomial regression both with and without these values, see Equation 5-1–5-4.*

The relationships are as follows:

Thermal conductivity, all values

$y = 27.265x^2 - 156.67x + 227.18$ R^2=0.88 Equation 5-1

Thermal conductivity, data from altered Äspö diorite excluded

$y = 48.822x^2 - 273.53x + 385.47$ R^2=0.94 Equation 5-2

Volumetric heat capacity, all values

$y = -2.5496x^2 + 15.156x - 20.215$ R^2=0.26 Equation 5-3

Volumetric heat capacity, data from altered Äspö diorite excluded

$y = 11.495x^2 - 60.971x + 82.891$ R^2=0.32 Equation 5-4

A comparison between the measured values and values calculated by Equation 5-1 and 5-3 are made in Table 5-1. There are some measured values that show large deviations from the results of the equations, as indicated in the table. The largest differences do not mainly coincide with the altered Äspö diorite, which motivates the use of the equations derived from all values (Equation 5-1 and 5-3).

Table 5-1. Comparison between measured values of thermal properties and values calculated by Equation 5-1 and 5-3.

Sample and depth (m)	Thermal Conductivity (W/m·K)			Volumetric heat capacity (MJ/m^3·K)		
	Measured	Calculated	*Difference*	Measured	Calculated	*Difference*
KA3539-1 1,0–1,22	2.42	2.41	*0.01*	2.22	2.20	*0.02*
KA3539-2 5,50–5,68	2.63	2.79	*–0.16*	2.14	2.14	*0.00*
KA3545 0,83–1,11	2.72	2.65	*0.07*	2.27	2.16	*0.11*
KA3551 0,95–1,15	2.76	2.72	*0.04*	2.15	2.15	*0.00*
KA3563 0,88–1,12	2.39	2.56	*–0.17*	2.15	2.18	*–0.03*
KA3569 0,87–1,20	2.42	2.56	*–0.14*	2.19	2.18	*0.01*
KA3575 1,03–1,27	2.44	2.44	*0.00*	2.18	2.20	*–0.02*
KA3581 1,10–1,33	2.50	2.41	*0.09*	2.32	2.20	*0.12*
KA3587 0,97–1,14	2.33	2.37	*–0.04*	2.29	2.21	*0.08*
KA3593-1 1,42–1,63	2.55	2.58	*–0.03*	2.10	2.17	*–0.07*
KA2599 G01 5,90–5,94	2.49	2.43	*0.06*	2.16	2.20	*–0.04*
KA2599 G01 14,63–14,67	2.34	2.41	*–0.07*	2.13	2.20	*–0.07*
KA2599 G01 25,32–25,36	2.47	2.50	*–0.03*	2.09	2.19	*–0.10*
KA2599 G01 44,28–44,32	2.99	3.21	*–0.22*	2.06	2.08	*–0.02*
KA2599 G01 50,10–50,14	3.58	3.65	*–0.07*	1.93	2.02	*–0.09*
KA2599 G01 61,89–61,93	3.68	3.50	*0.18*	2.02	2.04	*–0.02*
KA2599 G01 70,60–70,64	2.84	2.86	*–0.02*	2.10	2.13	*–0.03*
KA2599 G01 85,10–85,50	2.69	2.75	*–0.06*	1.96	2.15	*–0.19*
KA2599 G01 101.85–101.89	3.11	2.71	*0.40*	2.30	2.15	*0.15*
KA2599 G01 120,05–120,09	3.22	3.79	*–0.57*	1.99	2.00	*–0.01*
KA2599 G01 126,35–126,39	3.55	3.33	*0.22*	2.34	2.06	*0.28*
Mean			*–0.02*			*0.00*

The standard errors for the calculated values of thermal conductivity and volumetric heat capacity have been calculated. For the thermal conductivity, when all values are used, the standard error is 0.160. For volumetric heat capacity the standard error is 0.106 both with and without the values for altered Äspö diorite. This means that the correspondence between the model and the measured values is quite good.

5.2 Variation of thermal conductivity in boreholes

Equation 5-1 for thermal conductivity derived in section 5.1 is applied on density, determined every tenth centimetre in borehole KA3386A01 and KF0069A01. From this calculation, thermal conductivity for the boreholes is obtained.

However, the equations are only valid for the actual range of densities used to derive the equations, and for the actual rock types (diorite-granite) and REV (representative elementary volume). Therefore the equations are not valid when the density is outside the range used in the derivation. In the calculations the range has been expanded by 0.5% in each direction. Figure 5-2 and Figure 5-4 illustrate the thermal conductivity variations in the boreholes. Areas with density values outside the derived range are excluded from the graphs.

Figure 5-2 shows that most of the thermal conductivities in borehole KA3386A01 are low. In the section between 14 and 15 m, the density is too high to be used for this calculation. In other areas, mainly at 35–40, 43–46 and 49–50 m, the density is lower than the range for Equation 5-1. For borehole KF0069A01 only a few density values are outside the range for Equation 5-1, se Figure 5-4. The variation in thermal conductivity is larger for this borehole, with the values used. There are sections at different levels with a thermal conductivity around 2.5 W/(m·K) (Äspö diorite) and other sections where the conductivity is around 3.2 W/(m·K) (Ävrö granite). At the depth 35–42 m, the variation is even larger, which may indicate that the rock is inhomogeneous. Note that in the rock mapping legend no distinction has been made between Äspö diorite and Ävrö granite.

Variograms for the two boreholes is presented in Figure 5-3 and Figure 5-5, respectively. For KA3386A01 the variance increase slightly and smoothly when the lag length increases. This indicates that all data points are within the correlation distance from each other. The mean value of the thermal conductivity is roughly constant at 2.5 W/(m·K), with a few exceptions. For KF0069A01 the variance increases for small and large lag lengths. In between, around a lag length of about 10 m, the variance is almost constant. This pattern may depend on the groups of high and low values of thermal conductivity at different sections in the borehole.

The “nugget”, the intercept with the y-axis in Figure 5-3 and Figure 5-5 is the sum of small-scale variations and measurement errors.

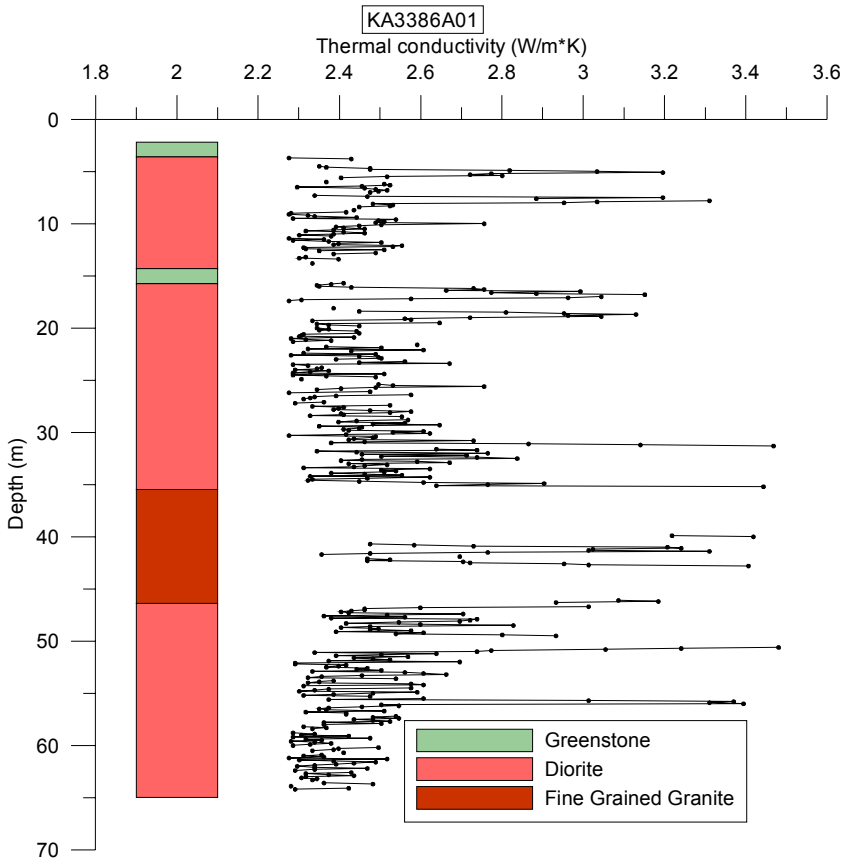

Figure 5-2. *Thermal conductivity vs. depth in borehole KA3386A01.*

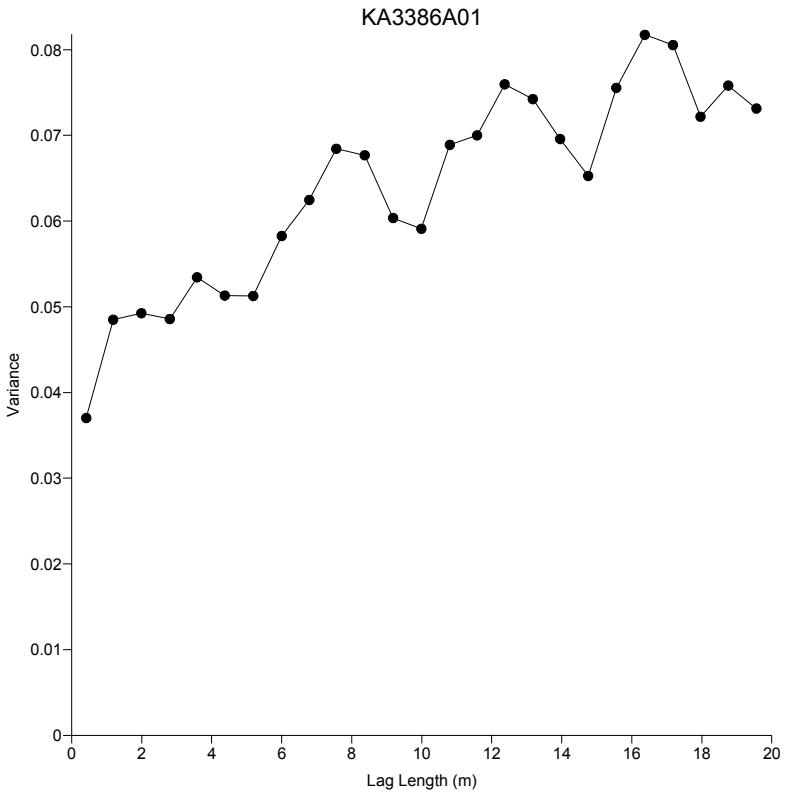

Figure 5-3. *Variogram of thermal conductivity for KA3386A01.*

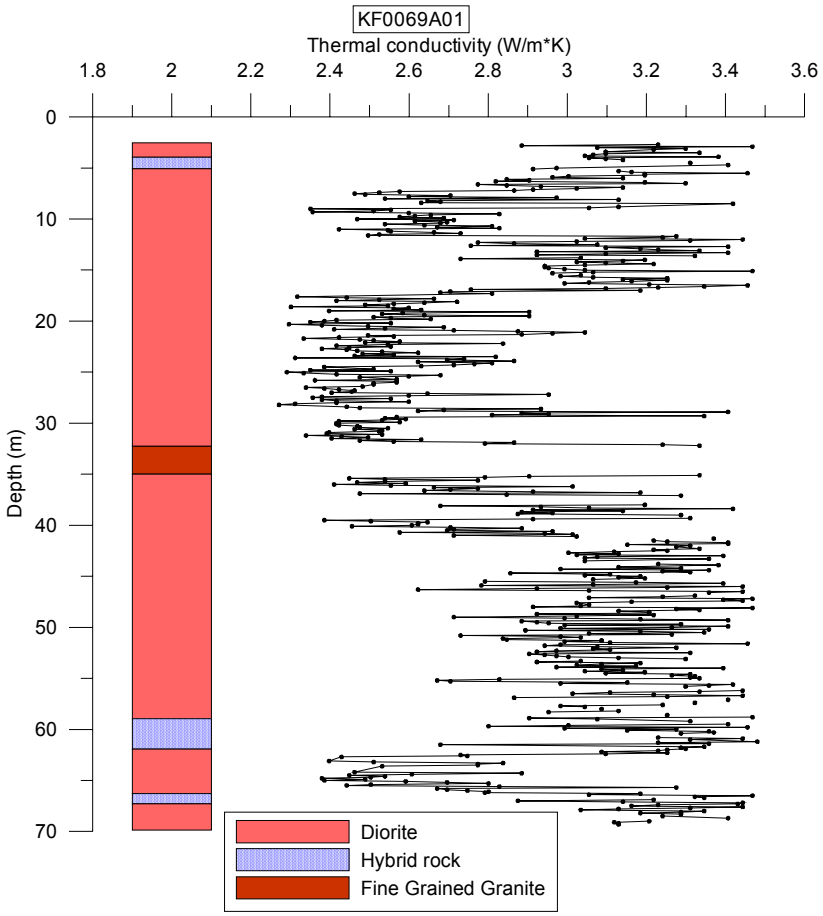

Figure 5-4. *Thermal conductivity vs. depth for borehole KF0069A01.*

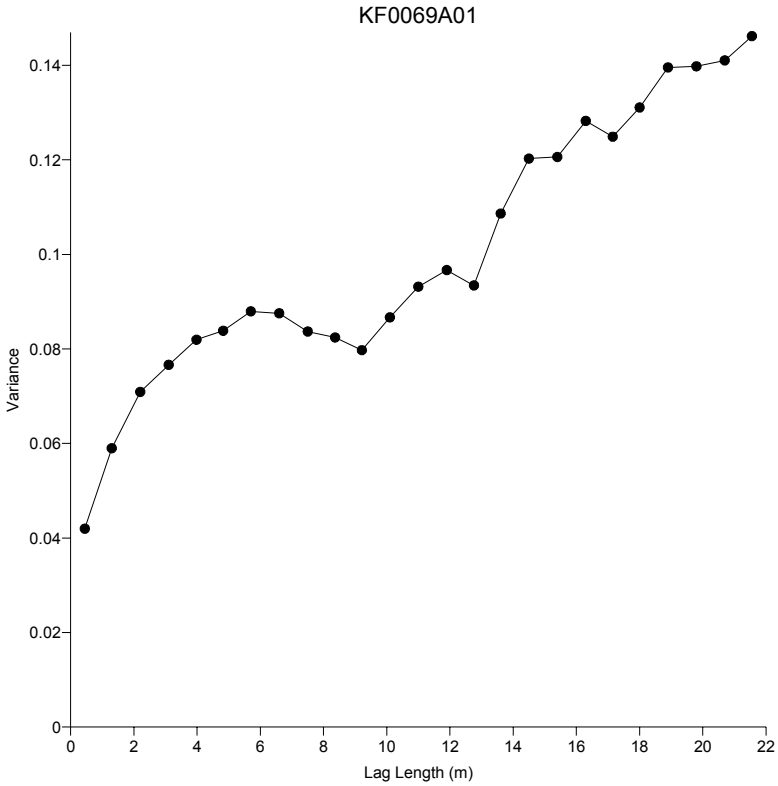

Figure 5-5. *Variogram of thermal conductivity for KF0069A01.*

6 Scales for thermal processes

6.1 Introduction

Rock forming minerals have different thermal properties, see /Horai, 1971/. The minerals exist in micro- or millimetre scale. Thus, there is a rather big variation in thermal properties in this scale. If the rock is fine grained, isotropic and homogeneous the properties have a large extent been averaged out in the cm-scale. Determination of thermal properties in laboratory is often made in this scale. However, even for a homogeneous rock type there is always a variation in properties due to chemical variations in the original magma. This variation can occur in the 1–100 m scale.

If the rock is anisotropic and inhomogeneous a larger variation exists in the small scale but not necessarily in the large scale.

The thermal function of a repository can be studied in different scales. In order to describe the influence from the natural climatic conditions on the ground surface, on the thermal conditions in a repository, some kind of mean value and deviation for the whole rock mass can be representative. To describe the thermal conditions around one single canister location, the thermal properties in the 1–10 m scale for the actual location is necessary. These thermal properties may not at all be representative for the whole rock mass.

Preliminary the following scales may be relevant:

- 0.0001–0.001 m for mineral analyses,
- 0.005–0.05 m for determination of thermal properties in laboratory,
- 1–10 m for the local thermal function of the canister,
- 10–100 m for the thermal function around the tunnel,
- 100–1000 m for the thermal function of the whole repository.

6.2 Sensitivity analyses for thermal processes in the canister scale

6.2.1 Introduction

The temperature field in the repository depends on thermal properties of the rock and the generated heat of the deposited canisters due to radioactive decay of the spent fuel. The layout of the repository is dependent on the temperature field. The design criterion is specified as the maximum temperature allowed on the surface of the canisters /Andersson et al, 2000/. Low thermal conductivity leads to a significantly larger distance between canisters than in the case of high thermal conductivity.

The sensitivity in canister temperature is highest for changes in the thermal properties for the area close to the canister. Therefore, it is of special interest to analyse the thermal impact on the canister for a variation in thermal properties in the rock mass in canister deposition scale, 1–10 m. In such a scale thermal steady-flux is established after a relative short period of time. When steady flux is established the heat capacity of the rock has a minor influence on the temperature.

6.3 Approach

In order to analyse the sensitivity in maximum canister temperature due to a variation in the thermal conductivity data, simulations has been made. The thermal process is modelled with the finite difference technique. The model assumes conductive thermal transport and symmetrical placement of tunnels and canister holes. For a closer description of the model and used analysis technique, see Appendix 2.

6.4 Simulations

The simulated area is symmetrical around a typical deposition hole (6·40 m) with non-flow boundaries (cc canister: 6 m, cc tunnels: 40 m), Figure 6-1.

Two different rock types, A and B, are assumed to exist in different areas. Each rock type has an assumed normal distribution of conductivities. The thermal conductivity is randomly distributed on small sub-volumes in each area. The thermal effect from the canister is 325 W/m (1625 W along 5 m borehole). The calculations of temperature are made for the canister deposition hole. The simulations have been performed by LTH, see Appendix 2 for details.

Two rock types, A and B, with normal distributed conductivities are supposed to exist:

	Thermal conductivity (W/(m·K))		Volumetric heat capacity ($MJ/(m^3 \cdot K)$)
	Average	Standard deviation	Average
Rock A:	3.4	0.28	2.16
Rock B:	2.6	0.15	2.16

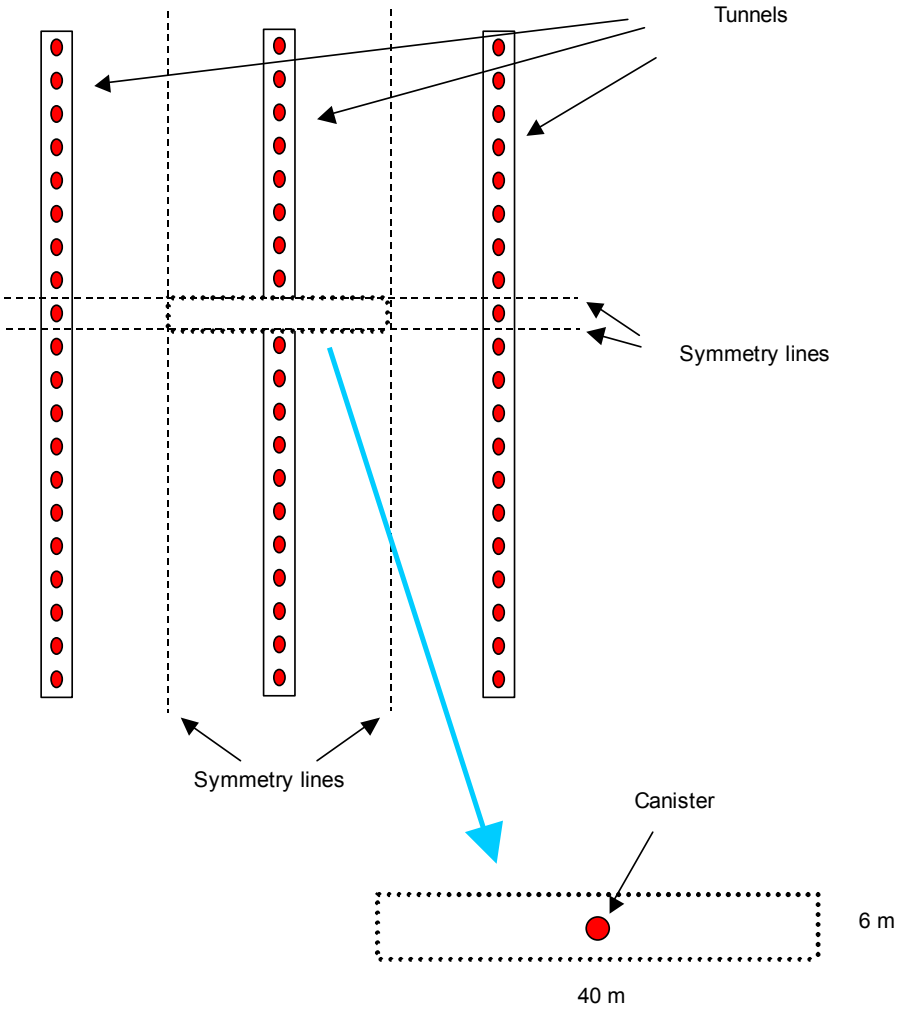

Figure 6-1. *Outline of tunnel system with canisters and studied geometry seen from above.*

6.4.1 Variation in the peripheral parts

The first simulation was used to investigate the influence on the deposit hole temperature of variations of thermal conductivity in the peripheral parts of the calculation area. In the peripheral part (D) a random value is used of the thermal conductivity for rock type B in each sub volume (cell). In the central part a constant mean value is used for rock type A.

The result shows that the influence on the temperature in the deposit hole is negligible even if the distance D is increased to 16 m and rock type A consequently only exists in the central 8 m.

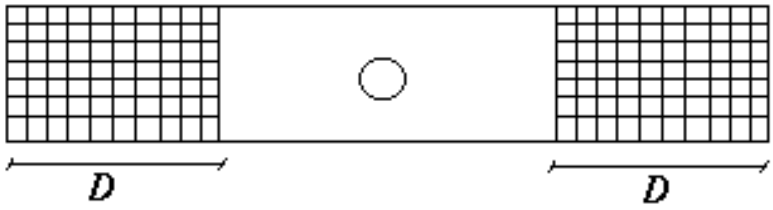

Figure 6-2. *Outline of studied geometry (6·40 m) with the canister (deposit hole) in the middle.*

6.4.2 Increasing fraction of rock species B

In this case rock type B exists in a successively increasing area described with the distance D in Figure 6-3. The rest of the area has the properties of rock type A.

At the simulation **one** random conductivity value for the distribution is used for each rock type and the temperature is calculated. This is repeated 100 times for each distance D and mean values and standard deviations for the temperature are calculated.

Figure 6-4 show the result of the calculations. The temperature is specified as a temperature difference between the calculated temperature and the temperature at a case with only rock type A (distance D=0).

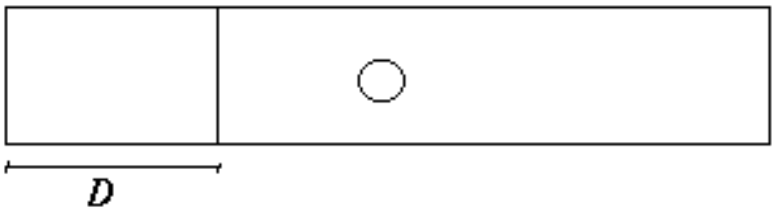

Figure 6-3. *Outline of studied geometry (6·40 m) with increasing area of rock B indicated with the distance D.*

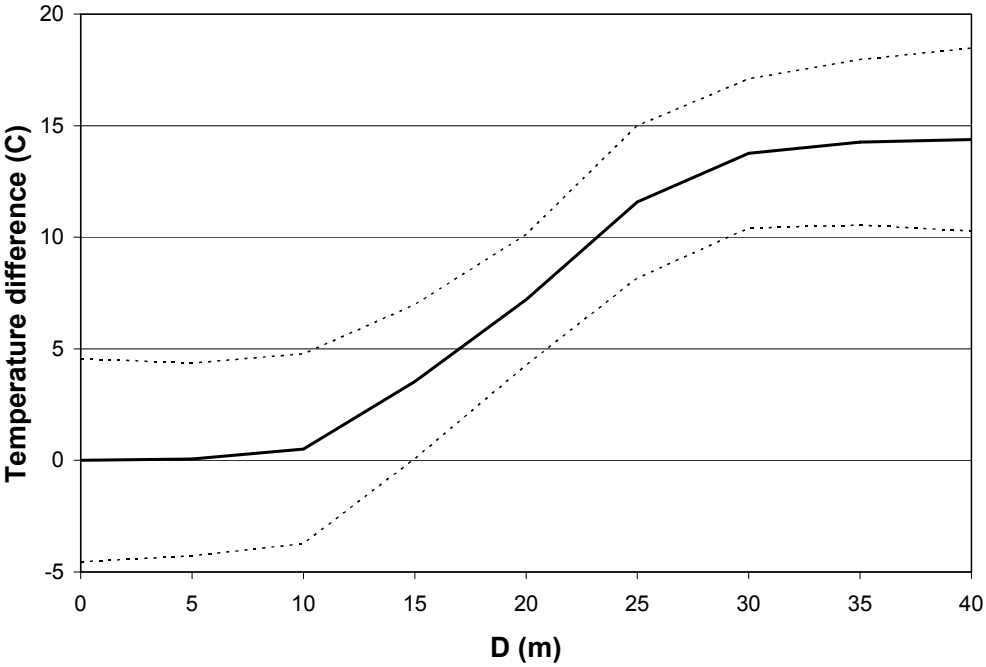

Figure 6-4. *Results for increasing fraction of rock species B, see Figure 6-3. The solid line shows the average value of the difference in steady-flux temperature compared to a situation where the considered calculation area consists of rock A with a homogeneous thermal conductivity of 3.4 W/(m·K). The dashed lines indicate the range contained within one standard deviation.*

The temperature difference is up to 14°C as mean value. The maximum temperature difference within 95% of the calculated temperatures (about 2 standard deviations) is about 32°C.

6.4.3 Increasing peripheral fraction of species B

The third simulation is similar to the latter but the distance D is successively increasing from both sides, see Figure 6-5. The result of the calculations is presented in Figure 6-6.

The temperature difference is up to 10°C as mean value when rock type B is increasing up to 17 m from both sides. The 6·6 m area closest to the canister consists of rock type A (with maximum increased rock B). The maximum temperature difference within 95% of the calculated temperatures (about 2 standard deviations) is about 25°C.

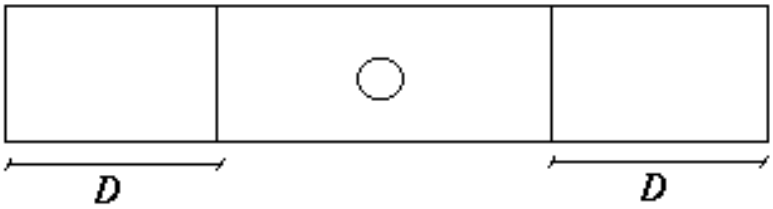

Figure 6-5. *Outline of studied geometry (6·40 m) for a case with increasing area of rock B on both sides, indicated with distance D.*

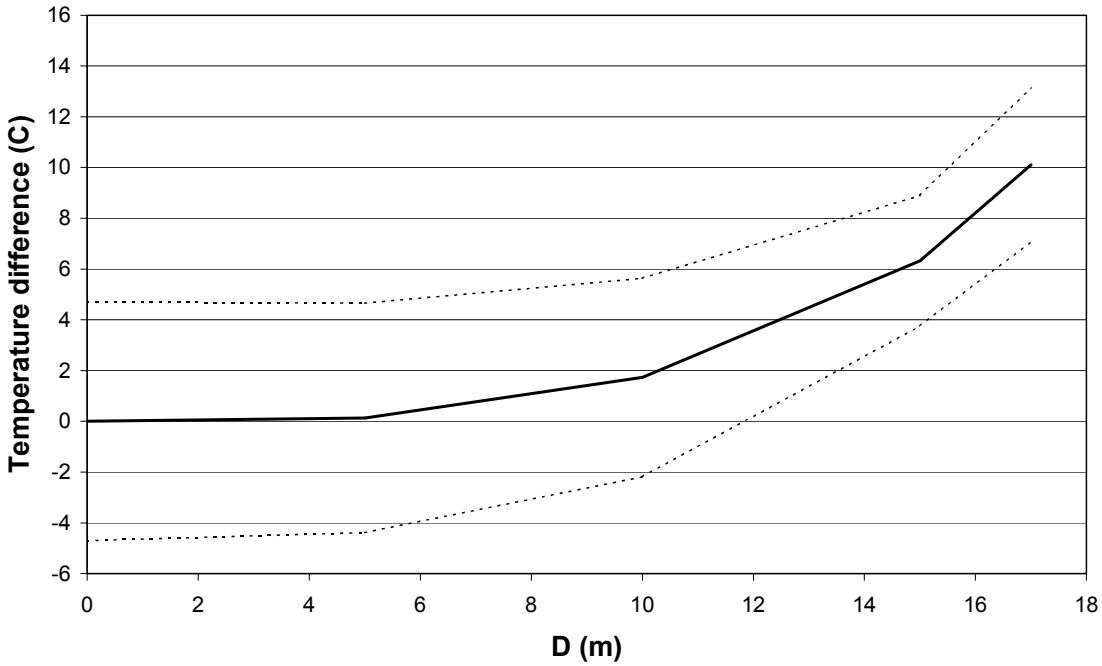

Figure 6-6. *Deposit hole surrounded by rock species A and increasing peripheral fraction of species B, Figure 6-5. The solid line shows the average value of the difference in steady-flux temperature compared to a situation where the calculation area consists of rock species A with a homogeneous thermal conductivity of 3.4 W/(m·K). The dashed lines indicate the range contained within one standard deviation (about 68% of the calculated temperatures).*

7 Evaluation

7.1 Thermal properties for the rock mass

7.1.1 Introduction

The investigations at Äspö HRL have been conducted since 1986. Slightly different systems for rock type designation have been used during the years. The result is that the database SICADA is not always consistent. In the mineral database the USGS rock type classification system has been used where the rock type is determined from the mineral content of the three dominating rock forming minerals; quartz, plagioclase and alkali feldspar (microcline). The local names on rocks used in the Äspö area are not included in the mineral database.

All rock mapping in tunnel and on drill cores is made in the local rock classification system, including Äspö diorite, Ävrö granite and Fine grained granite. However, in earlier performed rock mapping the name Smålands granite has mainly been used synonymously with Ävrö granite. Äspö diorite and Ävrö granite is hard to distinguish from each other by the eye. Besides mineral analyses, density measurement can also be used for identification. The most recently made rock mappings on drill cores at Äspö HRL are made at 350–500 m depth were the Äspö diorite is dominating. On these ocular rock mappings Ävrö granite is not mapped at all, only Äspö diorite. However, on revised mapping with density log or mineral analyses an occurrence of Ävrö granite exists (25–40%), see borehole KA2599G01 in Table 7-2 and borehole KF0069A01 in Figure 5-4**.**

The uncertainty in the rock type determination is time dependent due to different geologist and slightly different approaches. The uncertainty in the distinction between Äspö diorite and Ävrö granite is about 10–15% for mapping during tunnel construction and old core drilling. The uncertainty in the mapping of later core drilling is considerably higher /Stenberg, 2003/.

Another uncertainty is in giving the mineralogical composition of a porphyritic rock type from point counting of minerals. Furthermore, the investigated thin sections may not represent the rock in the actual core section.

These differences and uncertainties in the background material complicate the evaluation of the thermal properties of Äspö HRL.

7.1.2 Thermal properties of different rock types

The thermal properties of the rock mass at Äspö HRL have been analysed by different methods. The properties have been measured on 22 samples. The thermal properties have also been calculated from the mineral content for a much larger number of samples. With the method used to calculate the thermal conductivity from the mineral content, the thermal conductivity is underestimated, see 4.3.1. However, a correction can be made by using measured and calculated values from the same samples. This has been done for earlier investigations in Table 4-6. If the measured values are assumed to be correct, the geometric mean equation underestimates the thermal conductivity by 9–10% depending on the rock type. On the other hand the mineral content is overestimated with 1.4% (as a mean value). The total correction factor for the calculated

conductivities is therefore assumed to be 1.08. The exception is greenstone were no correction has been made due to the lack of measurements. The greenstone group is also inhomogeneous and consists of both volcanites and basic rock types.

In Table 7-1 a selection of groups of calculated thermal conductivities are compared to measured values for some different rock types at Äspö HRL. The Diorite group includes granodiorite, quartz monzodiorite etc and the rock classification is made from the mineral analyse and ocular mapping. The samples are collected at the surface, in the tunnel and from drill cores in the Äspö area. The Äspö diorite group, which mainly is a part of the diorite group, is classified from the original core mapping.

Table 7-1. Mean values of thermal conductivity (W/(m·K)) for different rock types. The calculated values are corrected (multiplicated with 1.08), except for greenstone.

Rock type	Calculated		Measured		Reference
	Number	Therm cond	Number	Therm cond	
All rock types	198	3.04	22	2.75	Table 4-3 and Table 3-1
Diorite	81	2.70	16	2.57	Table 4-3 and Table 3-3
Äspö diorite	37	2.58	16	2.57	Table 4-5 and Table 3-3
Ävrö granite (Smålands granite)	25	3.05	3	3.25	Table 4-5 and Table 3-3
Fine-grained granite	10	3.60	2	3.63	Table 4-5 and Table 3-3
Greenstone	27	2.82	–	–	Table 4-3

Which values we should have most confidence for can be discussed. However, there are a rather large number of measurements on Äspö diorite, which are in good agreement with calculated and corrected values. Therefore we can probably rely on these values a little more than the values for the diorite group. For the remaining groups it is suggested to rely more on calculated and corrected values due to the larger number of samples.

There are a number of uncertainties in calculated thermal properties from mineral composition:

- Uncertainties in the representativity of the sampling.
- Uncertainties in the point counting of minerals (modal composition).
- Uncertainties in reference values of thermal properties of different minerals.
- Uncertainties in the model for calculating the thermal properties of the rock sample.
- Uncertainties in rock type definition in Sicada database.

These uncertainties together with scale factors may cause possible systematic errors and larger variations in the results, compared to measurements.

7.1.3 Distribution of thermal properties

In order to create confidence intervals for the thermal conductivity, the data has been tested on different distributions. The data of calculated thermal conductivities is not in general normal or lognormal distributed, see chapter 4. The diorite group is closest to be normally distributed. Distribution free methods can also be used, but in general they require more observations and result in larger confidence intervals.

The spatial distribution of samples is concentrated to the ground surface, to bore holes and to the location of the tunnel. It is therefore very inhomogeneous, see Appendix 1.

7.1.4 Rock type distribution in the rock mass

In Table 7-2 the rock distribution according to different methods and depths is illustrated. The tunnel mapping and borehole mapping of KA2599G01 is ocular with support of mineral analyses in different points. The table shows that the distribution of rock types is depending on method and reference. For example the amount of greenstone is overestimated according to mineral analyses in Sicada compared to other references. This indicates that the sampling for mineral analyses may not have been random and the sampling probably not representative for the rock mass. The table also illustrates the difficulties to distinguish between Ävrö granite and diorite/Äspö diorite in the field or at the core mapping.

Table 7-2. Rock distribution according to tunnel mapping (approximately from /Rhén et al, 1997/), core mapping KA2599G01 /Sundberg, 2002/ and mineral analyses (LDV) (present study).

Rock type according to:	Rock type in %				Reference
	Äspö diorite	Ävrö granite	Fine grained granite	Green-stone	
Tunnel mapping, depth 200–300 m	55	24	14	7	/Rhén et al, 1997/
Tunnel mapping, depth 300–400 m	57	24	17	2	/Rhén et al, 1997/
Tunnel mapping, depth 400–500 m	93	0	4	3	/Rhén et al, 1997/
Borehole KA2599G01, Original core mapping depth 345–473 m	85		10	5	/Sundberg, 2002/
Borehole KA2599G01, revised mapping with support of mineral analyses, depth 345–473 m	60	25	11	4	/Sundberg, 2002/
Sicada: Original core mapping coupled to mineral analyses, depth 200–600 m	66[1]	11[2]	7	16	Present study
Sicada: Mineral analyses (LDV), depth 200–600 m	47[3]	29[4]		14	Present study

[1] Äspö Diorite, [2] Smålands Granite, [3] Diorite, [4] Granite.

7.2 Scale

7.2.1 Scales for observations and rock types

The sample scale for measurement of thermal properties in laboratory is about 0.5 to 5 cm. The scale for determination of mineral content from point counting is much smaller. This implies that the variation in thermal properties determined from the mineral content should be larger than from measurement. However, for Äspö diorite the standard deviation is almost the same for both measured and calculated values. The number of observations is however higher for calculated values.

The diagrams and variograms for calculated thermal conductivity from density loggings (Figure 5-2 – Figure 5-5) indicate a small-scale variation. However, it is unclear if the variation caused by real thermal conductivity variations or by effects of measurement uncertainties in the density logging.

The diagrams with thermal conductivity versus depth indicate blocks of Ävrö granite in the Äspö diorite with the size 5–20 m.

In order to investigate a possible correlation scale for thermal properties of different rock types, variograms have been used. Data was collected from the database of calculated thermal conductivities from mineral analyses in Sicada. In general no conclusions about correlation distance could be drawn, probably due to few samples and an uneven spatial distribution. For diorite (LDV) in both 2D and 3D a tendency to a limit for correlation was indicated at about 200–300 m, see Appendix 1.

7.2.2 Sensitivity of thermal process in canister scale

The temperature at the canister deposit hole is not sensitive to small-scale variations of the thermal conductivity in the peripheral areas.

The simulations of different rock types in the canister-tunnel scale indicate a medium and maximum canister hole temperature difference of 14 and 23ºC respectively due to the presence of diorite instead of granite. The latter temperature difference depends on the confidence interval of calculated temperatures. In this case about a 68% confidence interval is chosen (one standard deviation).

Within the same rock type the temperature difference can be about ±5ºC from the mean value with 68% confidence.

If two rock types exist, one in the area closest to the canister and the other in the peripheral area, the simulations indicate a rather high temperature influence compared to the case with one rock type. Thus, in the case with a high thermal conductive rock in the tunnel area it is still possible to have a quite large influence on the canister temperature from a low conductive rock outside the tunnel area.

However, the maximum temperature range is overestimated if a part of the distribution in thermal conductivities is related to small-scale variations, which have negligible effect on the calculated temperatures. If, for example, half of the standard deviation is related to such small-scale variations, the maximum temperature interval is related to 95% confidence limit. However, as discussed in chapter 7.2.1, the knowledge of thermal conductivity variations in different scales is limited.

8 Conclusions and recommendations

8.1 Conclusions

8.1.1 Thermal conductivity values

Calculations of thermal conductivity of rock types from mineral analyses in Sicada, and corrected for possible errors, give values of 2.6 (std: 0.17) W/(m·K) for Äspö diorite and 3.05 (std: 0.32) W/(m·K) for Ävrö granite. The sample values for both rock types are not normally or log normally distributed. The standard deviation may be overestimated due to scale factors. The determination has uncertainties in the representativity of sampling, the modal analysis, reference values of minerals, the calculation model, and the rock type definition in Sicada.

The heat capacity, estimated from measurements, is 2.16 (std: 0.09) MJ/(m^3·K) for Äspö diorite and 2.06 (std: 0.19) MJ/(m^3·K) for Ävrö granite.

The canister temperature is more sensitive to the thermal conductivity than to the heat capacity. This is partly due to larger parameter sensitivity for thermal conductivity in the thermal process and actual geometry. However, the main reason is larger variation interval for thermal conductivity.

Measurements of thermal properties are preferable to calculations from mineralogical composition due to less uncertainty.

8.1.2 Rock classification

There are uncertainties in the base material of rock classification, mainly due to problem to distinguish between Äspö diorite and Ävrö granite but also because of different classification system. From a thermal point of view the uncertainties and differences in rock type definition in the Äspö HRL raise the question if it is meaningful to define rock types more precisely than what can be done by ocular mapping. There is no need for a more precise rock type definition than at a level that can be used to determine the spatial distribution of the rock.

8.1.3 Density logging

The measured densities show a good correlation with thermal properties for the dominating rock types at Äspö HRL (Äspö diorite, Ävrö granite and Fine grained granite). Density logging seems to be a useful method to define the spatial distribution of thermal properties in the rock mass. However, it demands a good calibration between thermal conductivity and density, routines to handle rock types that do not fit the model, and well defined criteria when it should not be used. Furthermore the model needs to be tested on rock types at other locations.

8.1.4 Scale

There is an insufficient knowledge in the variation of thermal properties at different scales. If the whole variation within a rock type is in the cm-m scale the thermal influence on the canister is small. This is due to the fact that the small-scale variation in thermal properties is mainly averaged out in the 5–10 m scale. If the main variation within rock types is in the 5–10 m scale there is probably a significant effect on the canister temperature. However, it is likely that the observed variation occurs in both these scales.

In the thermal data simulations the observed standard deviations of thermal conductivity for each rock type have been used. A part of this deviation is probably due to small-scale variations that are averaged out in the simulation scale. The range of temperatures is therefore probably overestimated.

The simulation result shows that the temperature of the canister hole is influenced by the thermal properties in a 6·40 m^2 area around the canister. The influence is stronger closer to the canister. Variations in thermal properties (assumed normally distributed) within one example of rock type give the temperature variation ±5ºC with 68% confidence. If, for example, half of the standard deviation is assumed to be in the small scale, the confidence is instead 95%.

With high and well defined thermal properties in the tunnel area there is still a large influence on canister temperature if low conductive rock is present outside the tunnel. The thermal behaviour in canister-tunnel scale is more influenced by variations in the thermal conductivity than in the heat capacity.

8.2 Recommendations

Calculations of the thermal properties from modal analyses have uncertainties. Direct measurements are recommended.

Density logging seems to be a promising method to evaluate the spatial distribution, scale factors and the variations in thermal properties of the rock mass. A model needs to be developed in order to handle different rock types, variations (including alterations) in mineral composition and both low and high density and porosity zones, outside of the common range.

A better knowledge is required about scale effects on thermal properties due to the measurement process and the actual thermal process in canister-tunnel scale. Measurements of thermal properties in different scales are needed. More extensive simulations to study the thermal influence on the canisters are also recommended.

9 References

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Histograms

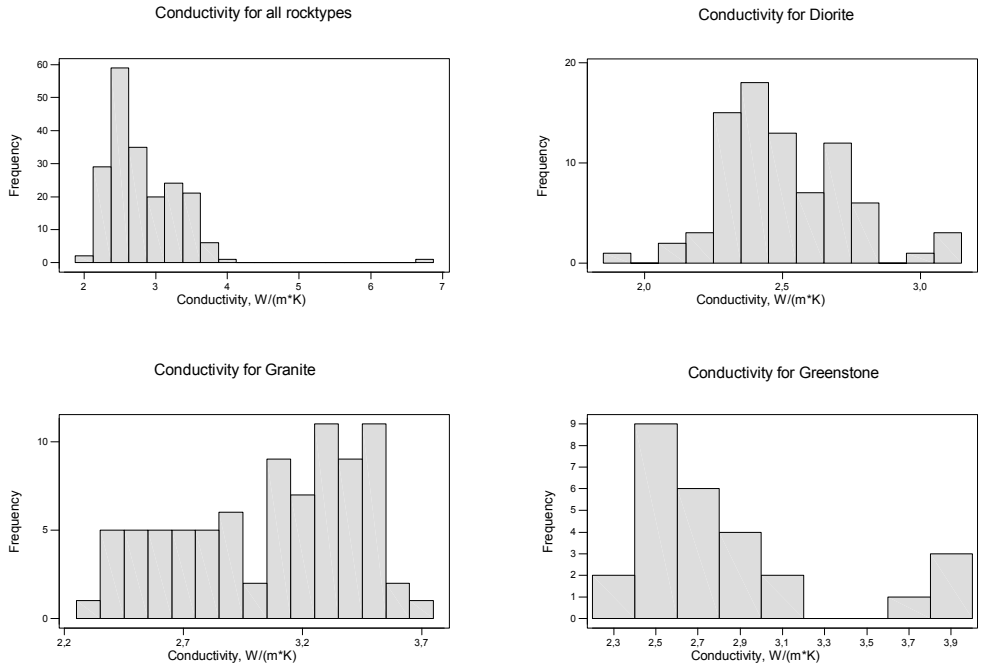

Figure A1-1a, b, c and d. *Histogram over thermal conductivity W/(m·K), for all rock types, diorite, granite and greenstone, respectively.*

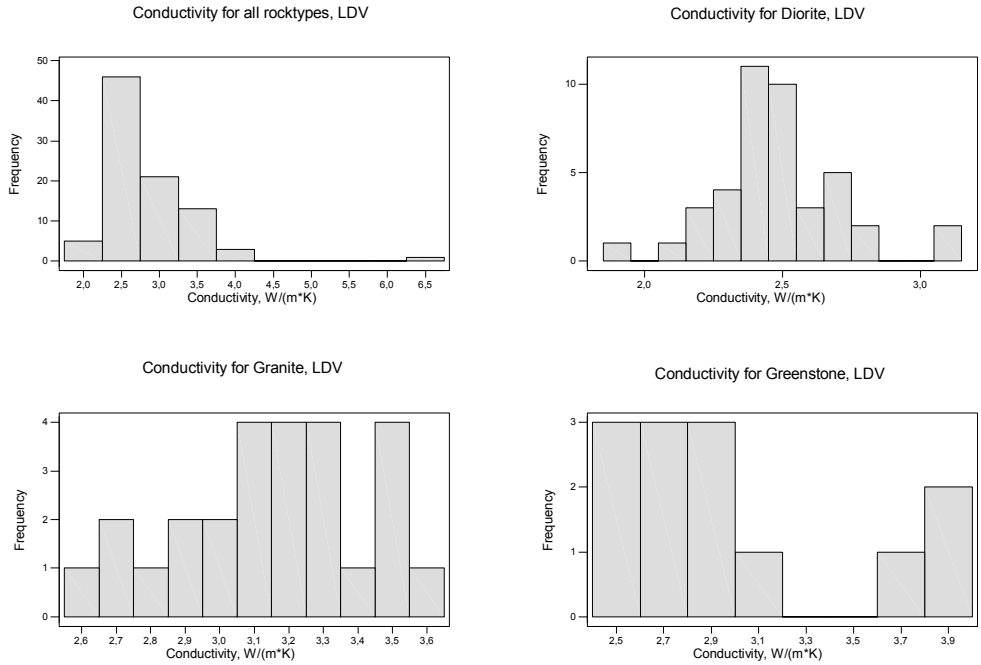

Figure A1-2a, b, c and d. *Histogram over thermal conductivity W/(m·K), for all rock types, diorite, granite and greenstone, respectively, Limited Data Volume.*

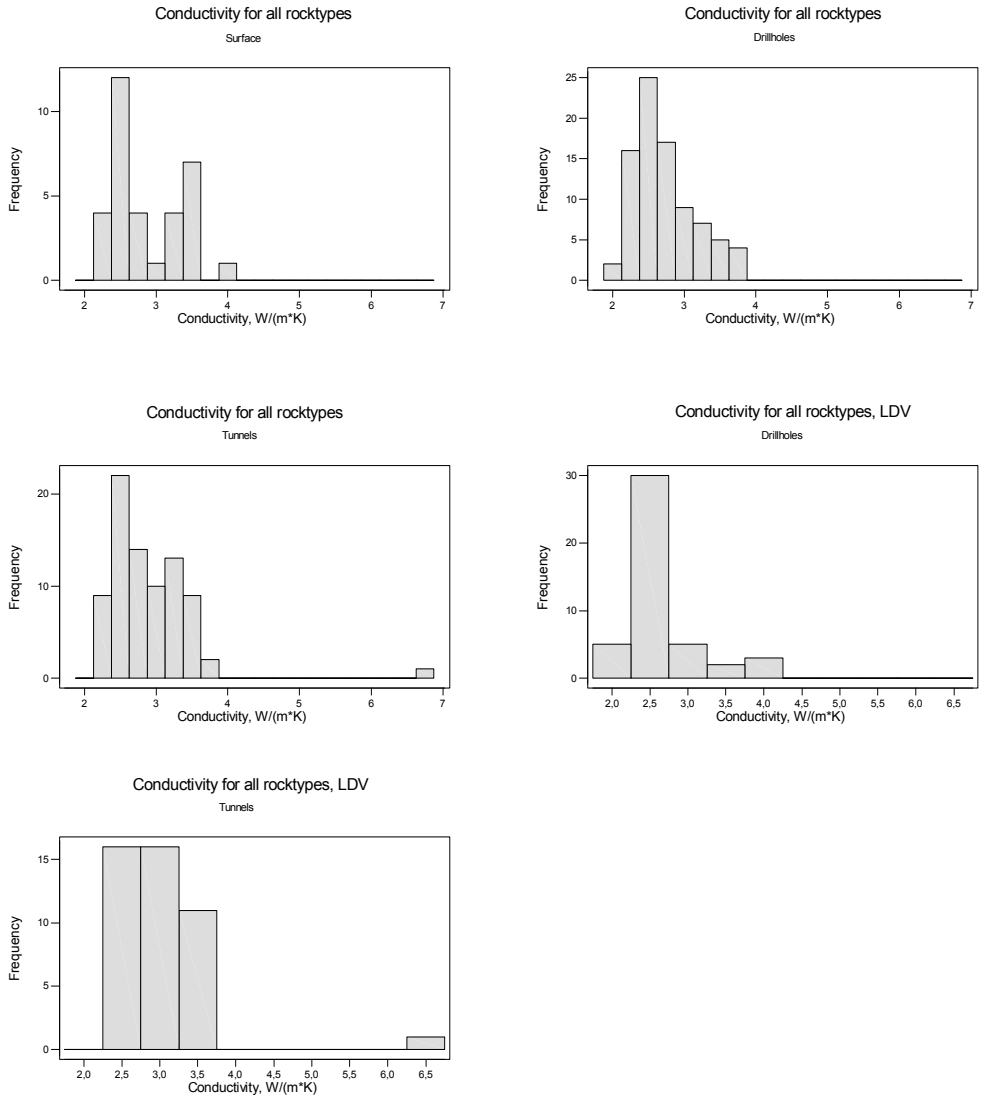

Figure A1-3a, b, c, d and e. *Histogram over thermal conductivity W/(m·K), for all rocktypes, surface-samples, drillhole samples, tunnel samples, drillhole samples, Limited Data Volume, and tunnel-samples, Limited Data Volume, respectively.*

Normal probability plot

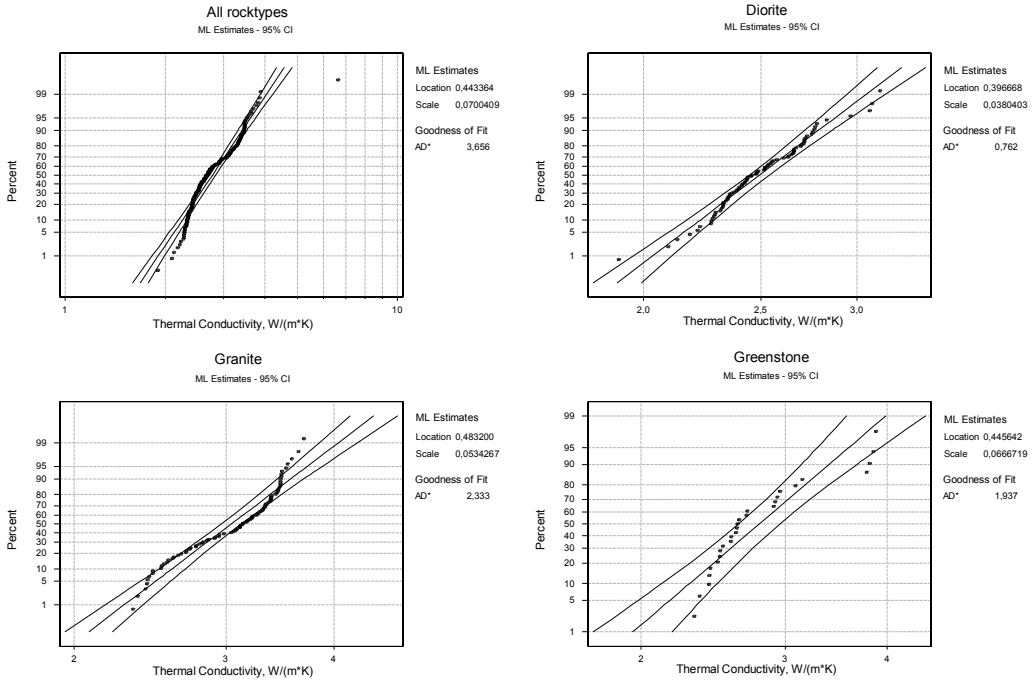

Figure A1-4a, b, c and d. *Lognormal base 10 Probability Plot for Thermal Conductivity W/(m·K), all rock types, diorite, granite and greenstone, respectively. "ML Estimates" is an estimation method called Maximum Likelihood. "95% Cl" means 95% confidence level.*

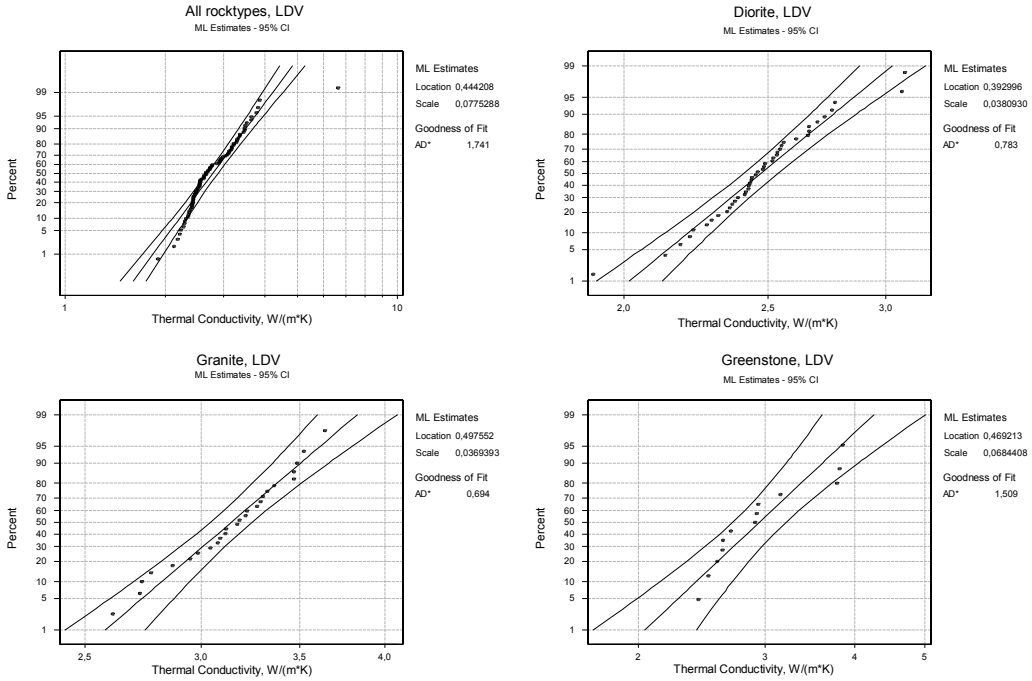

Figure A1-5a, b, c and d. *Lognormal base 10 Probability Plot for Thermal Conductivity W/(m·K), all rock types, LDV, diorite, LDV, granite, LDV and greenstone, LDV, respectively. "ML Estimates" is an estimation method called Maximum Likelihood. "95% Cl" means 95% confidence level.*

Geometric distribution

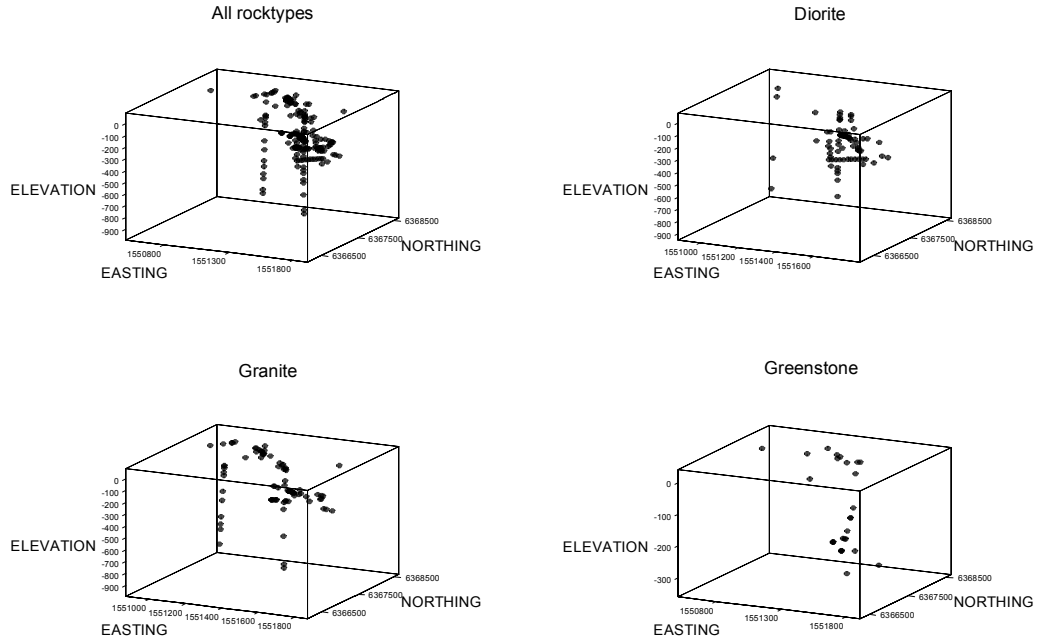

Figure A1-6a, b, c and d. *Sample distribution diagram for all rock types, diorite, granite and greenstone, respectively.*

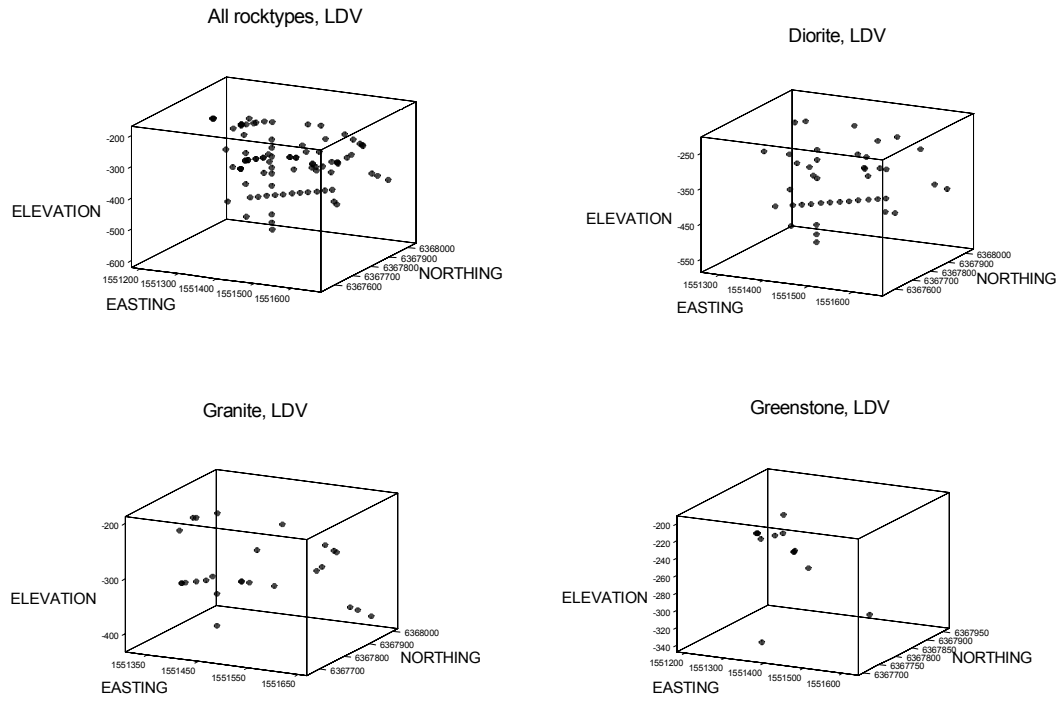

Figure A1-7a, b, c, and d. *Sample distribution diagram for all rock types, diorite, granite and greenstone, respectively, Limited Data Volume.*

Variograms in 2 dimensions

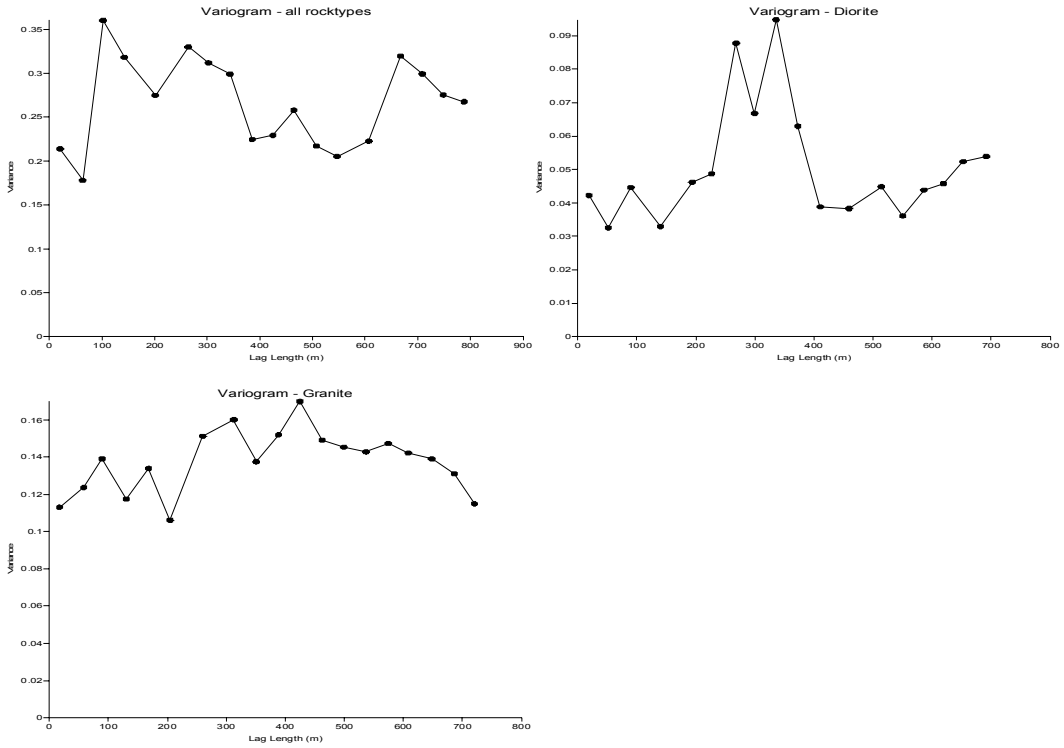

Figure A1-8a, b, and c. *Variance at different lags for all rock types, diorite, granite and greenstone, respectively– 2 dimensions.*

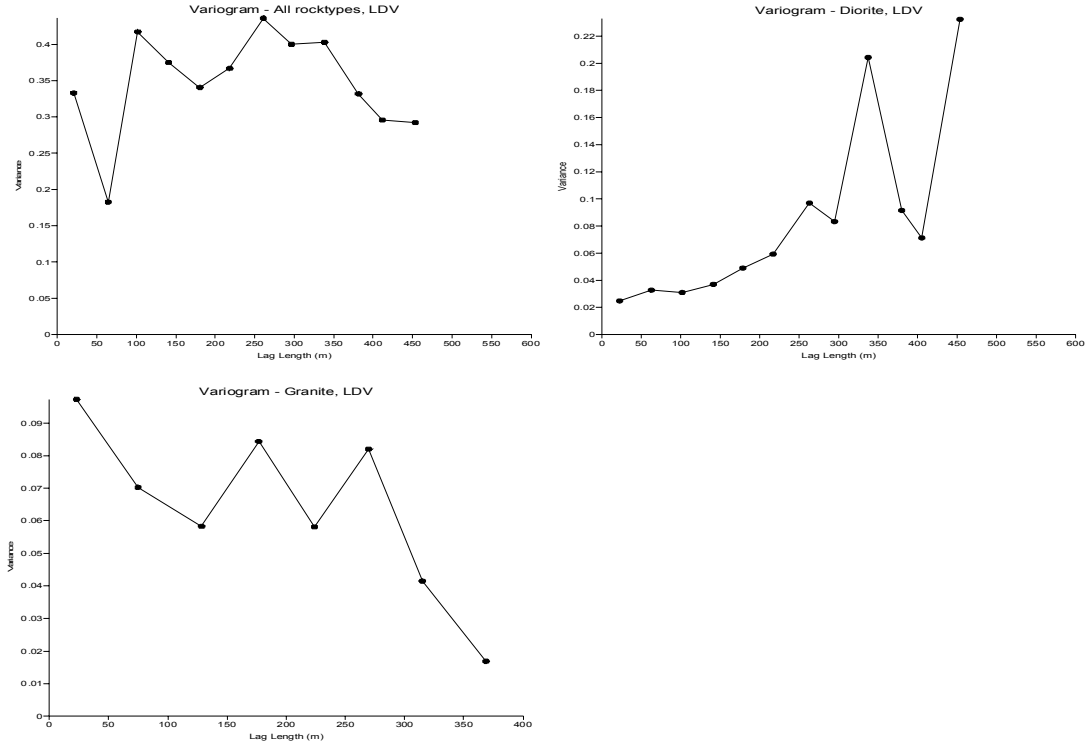

Figure A1-9a, b, and c. *Variance at different lags for all rock types, diorite, granite and greenstone, respectively – 2 dimensions, Limited Data Volume.*

Variograms in 3 dimensions

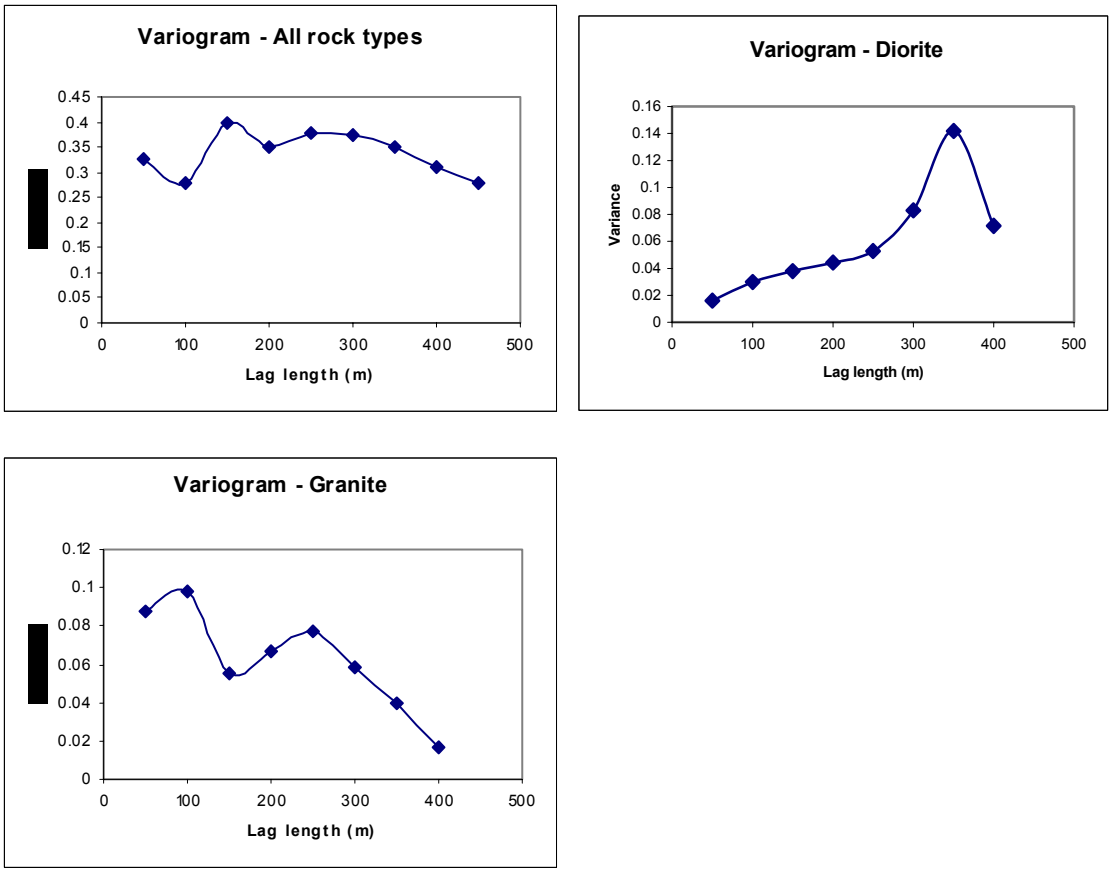

Figure A1-10a, b and c. *Variance at different lags for all rock types, diorite, granite and greenstone, respectively – 3 dimensions, Limited Data Volume.*

Simulering av inverkan av inhomogena termiska egenskaper i närområdet av kapselförvarshål

Simulation of the influence of inhomogeneous thermal properties in the vicinity of a radioactive waste repository

Abstract

The aim of this study is to show how the maximum temperature at the canisters is influenced by a variation of the rock thermal properties in the vicinity of the waste repository. The thermal process has been simulated with use of a model based on the finite difference method (FDM). The model assumes conductive heat transfer in the rock mass and symmetrical location of canisters and tunnels. The considered region is bounded by symmetry planes. The temperature difference between the canister and average temperature in the considered region is calculated at "steady-flux" conditions. The rock thermal conductivities in this region are assigned randomly based on an assumed statistical normal distribution. Three idealized situations outlined in Figures A2-3, A2-4, and A2-6 are considered. The calculations are performed 100 times with random thermal conductivities for each set of parameter values and the mean value and standard deviation of the resulting distribution of steady-flux temperatures are evaluated.

Introduktion

Studien avser att belysa hur maximal temperatur vid kapselförvarshål påverkas av variation av bergets termiska egenskaper i förvarshålets närområde. Den termiska processen simuleras med hjälp av finita differens teknik (FDM). Modellen antar konduktiv värmeledning i bergsmassan och förutsätter en symmetrisk placering av förvarshål och tunnlar. Simuleringen utförs på ett av symmetriplan avgränsat område. I detta område fördelas termiska egenskaper slumpmässigt på mindre delvolymer enligt känd eller antagen frekvensfördelning avseende bergart och termiska egenskaper. Delvolymernas storlek varieras för att undersöka inverkan av representativ skala för inhomogeniteterna.

Analysmetod

Värmetransporten i berget antas sker genom konduktiv värmeledning i ett horisontellt plan beskrivet med ett kartesiska koordinater x och y. Bergstemperaturen T variation med tiden t beskrivs av värmeledningsekvationen.

$$-\frac{\partial}{\partial x}\left(-\lambda\frac{\partial T}{\partial x}\right)-\frac{\partial}{\partial y}\left(-\lambda\frac{\partial T}{\partial y}\right)=\rho c\frac{\partial T}{\partial t}$$

Värmeledningsförmågan $\lambda(x,y)$ i berget antas vara isotrop och variera rumsligt med x och y. Bergets densitet ρ och specifika värmekapacitet c antas vara homogena.

Förvarshålet är cylinderformat med vertikal symmetriaxel, vilken är belägen vid x=0 och y=0. Det betraktade området kan av symmetriskäl antas vara begänsat till:

$-l_x < x < l_x \;\; -l_y < y < l_y$

Vid beräkningsområdets ränder sätts värmeflödet till 0 på grund av symmetriskäl. Detta villkor antas vara uppfyllt även om värmeledningsförmågan rumsligt inte är symmetrisk med avseende på förvarshålet.

Initiellt har berg och förvarshål i en homogen temperatur T_0 i det betraktade horisontella planet.

I förvarshålet avges en värmeeffekt q_0 (W/m) som avtar långsamt med tiden. Detta medför att beräkningsområdets medeltemperatur T_m med tiden t ökar som:

$$T_m(t)=T_0+\frac{q_0 t}{4\rho c l_x l_y}$$

I denna studie är avsikten inte att analysera hur egenskaperna i förvarshålets inre och dess omedelbara närhet påverkar den termiska processen. Den tillförda effekten ger, oberoende av förvarshålets utformning, efter en kort tid en relativt stationär temperaturdifferens mellan förvarskapseln och en cirkelyta runt förvarshålet. Denna cirkelyta har valts till en radie på 1,22 m från borrhålets axel (Borrhålets radie är 0,875 m). I de betraktade beräkningsfallen antas förvarshålets termiska egenskaper vara desamma, vilket innebär att den temperaturdifferens som uppstår mellan kapsel och cirkelytan blir lika för olika fall. Analysen redovisar skillnader i temperaturutvecklingen.

Med adiabatiska randvillkor och konstant värmekälla inträder efter en viss tid ett tillstånd, s.k. steady-flux, där värmeflödet i beräkningsområdet blir stationärt och temperaturen ökar linjärt med tiden i varje punkt /Claesson och Probert, 1996; Probert och Claesson, 1997/. Vid detta tillstånd blir temperaturskillnaden mellan förvarshålet och beräkningsområdets medeltemperatur konstant. ”Steady-flux”-temperaturskillnaden för ett rektangulärt område kan skrivas:

$$T_{sf}=\frac{q_0}{2\pi\lambda}\left[\ln\left(\frac{l_y}{\pi r_b}\right)+\frac{\pi l_x}{6 l_y}\right]$$

Här är r_b förvarshålets radie.

En karakteristisk tid *t* för steady-flux-tillståndets insvängningsförlopp ges av:

$$\frac{\lambda t}{\rho c l_x^2} = \frac{3}{\pi^2} \approx 0,076$$

Med gällande ingångsdata erhålls för värmeledningsförmågan 3,4 W/m,K en karakteristisk tid på 2,4 år och för 2,6 W/m,K blir denna tid 3,1 år. I de redovisade beräkningarna har den termiska processen simulerats i 2500 dagar, vilket är 6,8 år. Under denna tidsperiod kan avgiven värmeeffekt betraktas som en konstant.

Värmeledningsförmågan för en bergart antas vara normalfördelad med medelvärdet λ_m och standardavvikelsen σ enligt:

$$f(\lambda) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\lambda-\lambda_m)^2}{2\sigma^2}}$$

Kumulativ frekvens Φ(λ) ges av:

$$\Phi(\lambda) = \int_{-\infty}^{\lambda} \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(\lambda'-\lambda_m)^2}{2\sigma^2}} d\lambda'$$

Numerisk modell

Värmeledningsproblemet simuleras med en finita differensmetod (FDM). Beräkningsområdet delas in ett antal kvadratiska eller rektangulära celler. Det cylindriska förvarshålet approximeras med ett antal celler som tillsammans har samma tvärsnittsarea som förvarshålet.

Värmeeffekten tillförs de beräkningsceller som är belägna centralt i förvarshålet (en detaljerad beskrivning av förvarshålets egenskaper är inte nödvändig för denna analys).

Värmeledningsförmågan för en bergart är normalfördelad enligt ovan. Vid simulering tilldelas olika delområden ett värde på värmeledningsförmågan, vilket går till så att ett värde mellan 0 och 1 motsvarande kumulativ frekvens Φ(λ) erhålls genom slumptals-generering. Med utgångspunkt från detta värde kan sedan värmeledningsförmågan bestämmas.

Den numeriska modellen har validerats mot den analytiska ”steady-flux”-lösningen för ett homogent material.

Grunddata

Följande grunddata har använts vid beräkningen:

l_x	20 m
l_y	3 m
r_b	0,875 m
ρc	2,16 MJ/m^3,K
P	1625 W eller 325 W/m

Två bergarter, A och B, antas förekomma:

Rock species	Average	Standard deviation
A	3,4	0,28
B	2,6	0,15

Kumulativ frekvens för dessa bergarter visas i figur A2-1 och A2-2.

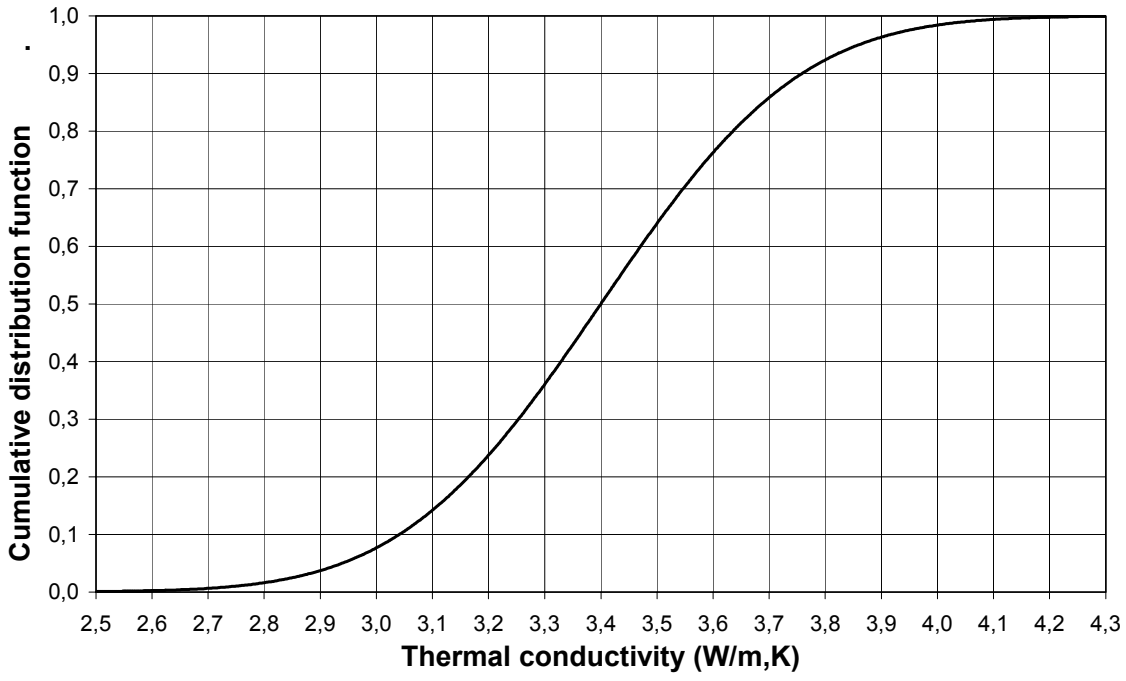

Figure A2-1. *Cumulative distribution function $\Phi(\lambda)$ for the thermal conductivity of rock species A.*

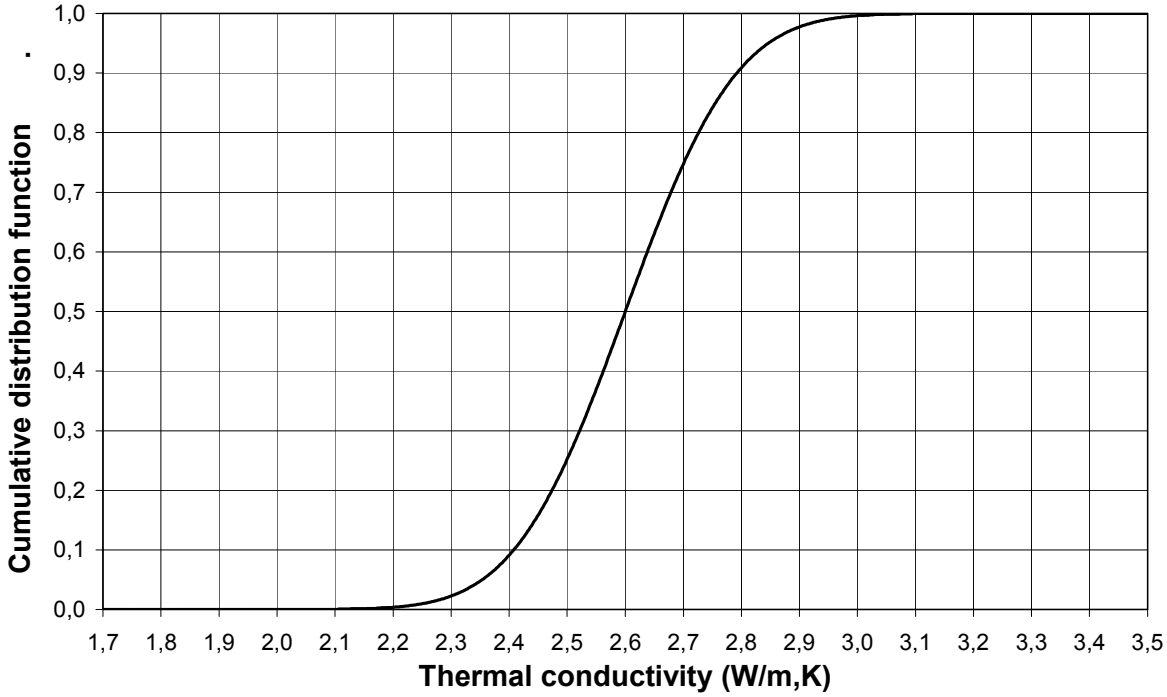

Figure A2-2. *Cumulative distribution function $\Phi(\lambda)$ for the thermal conductivity of rock species B.*

Resultat

Fall A. Perifer variation av värmeledningsförmågan

Detta fall avser att belysa inverkan av varierande värmeledningsförmåga i beräkningsområdets perifera delar. Delvolymerna är kvadratiska med sidlängden 0,4 m. Se figur A2-3. I de två perifera delarna ansätts ett slumptalsgenererat värde på värmeledningsförmågan för bergart A i varje delområde. I den centrala delen kring är värmeledningsförmågan lika med 3,4 W/m,K.

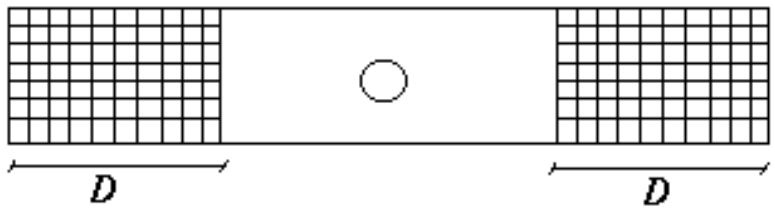

Figure A2-3. *Outline of studied geometry in case A.*

Beräkningsresultatet sammanfattas i tabell A2-1. Det framgår att inverkan på förvarshålets temperatur är obetydlig både vad avser medelvärde och standardavvikelse.

Table A2-1. Peripheral variation of rock thermal conductivity.

D (m)	Average	Standard deviation
0	50,196	–
8	50,088	0,014
12	50,125	0,043
16	50,198	0,091

Fall B. Ökande andel av bergart B

I detta fall förekommer bergart B med en utsträckning markerat med avståndet D enligt figur A2-4. Det övriga området har värmeledningsförmågan för bergart A. I övrigt ”Steady-flux”-temperaturen anges som en skillnad mot det fall då hela beräknings-området består av bergarten A med värmeledningsförmågan 3,4 W/m,K.

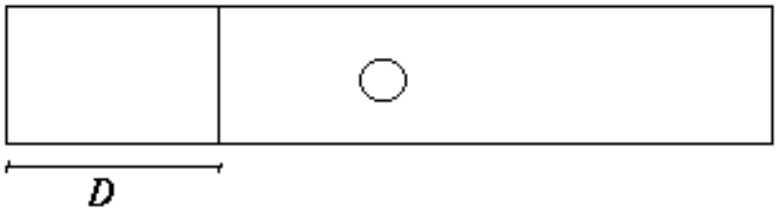

Figure A2-4. *Outline of studied geometry in case B. Rock species B occurs in the area marked with the distance D.*

Vid simuleringen ansätts **ett** slumptalsbaserat värde (se ovan) för vardera bergart A och B i de två delområden och ”steady-flux”-temperaturen beräknas. Detta upprepas 100 gånger för varje värde på D varefter medelvärde och standardavvikelse σ för ”steady-flux”-temperaturen beräknas. Medelvärde av T_{sf} och temperaturen $T_{sf}-\sigma$ och $T_{sf}+\sigma$ som funktion av avståndet D visas i figur A2-5. Notera att 15% av beräknade värden på T_{sf} är större än $T_{sf}+\sigma$, men att endast 2% är större än $T_{sf}+2\sigma$.

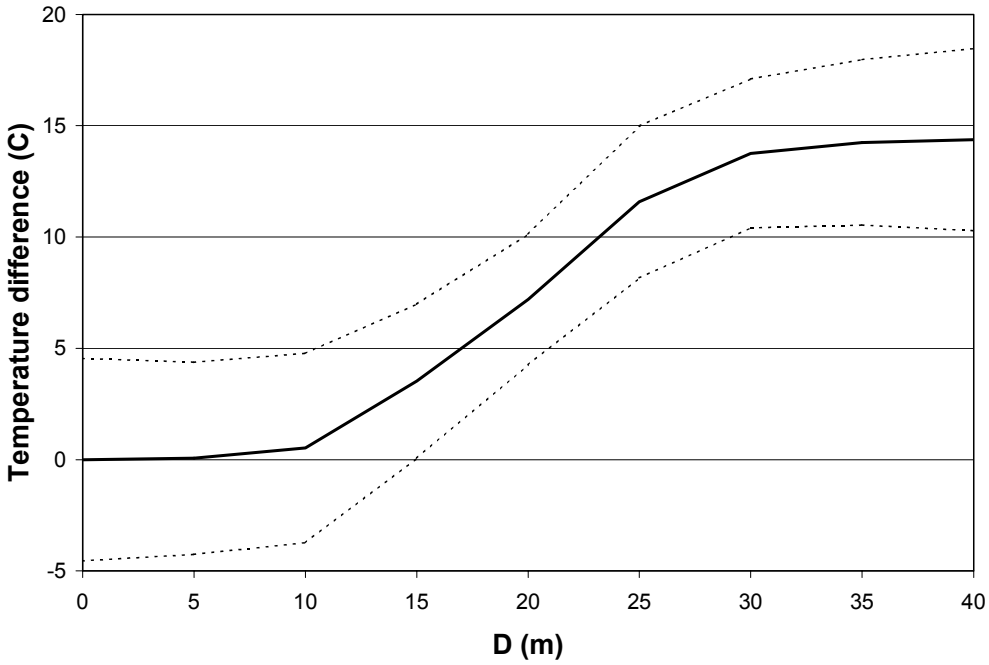

Figure A2-5. *Case B. Increasing fraction of rock species B. See Figure A2-4. The solid line shows the average value of the difference in steady-flux temperature compared to a situation where the considered calculation area consists of rock species A with homogeneous thermal conductivity of 3,4 W/m,K. The dashed lines indicate the standard deviation.*

Fall C. Förvarshål omgivet av bergart A. Perifert ökande andel av bergart B

I detta fall förekommer bergart B med en utsträckning markerat med avståndet D enligt figur A2-4. Området kring förvarshålet har värmeledningsförmågan för bergart A. ”Steady-flux”-temperaturen anges som en skillnad mot det fall då hela beräknings-området har består av bergarten A med värmeledningsförmågan 3,4 W/m,K.

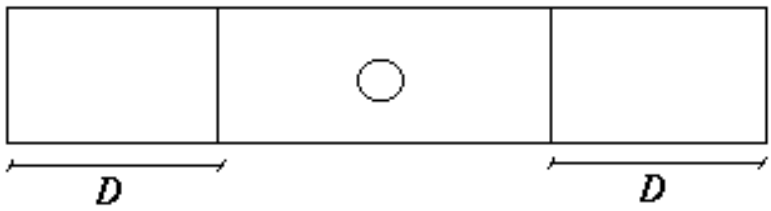

Figure A2-6. *Outline of studied geometry in case C. Rock species B occurs in the areas marked with the distance D.*

Vid simuleringen ansätts **ett** slumptalsbaserat värde (se ovan) för vardera bergart A och B i de två delområden och ”steady-flux”-temperaturen beräknas. Detta upprepas 100 gånger varefter medelvärde och standardavvikelse för ”steady-flux”-temperaturen beräknas. Se figur A2-7.

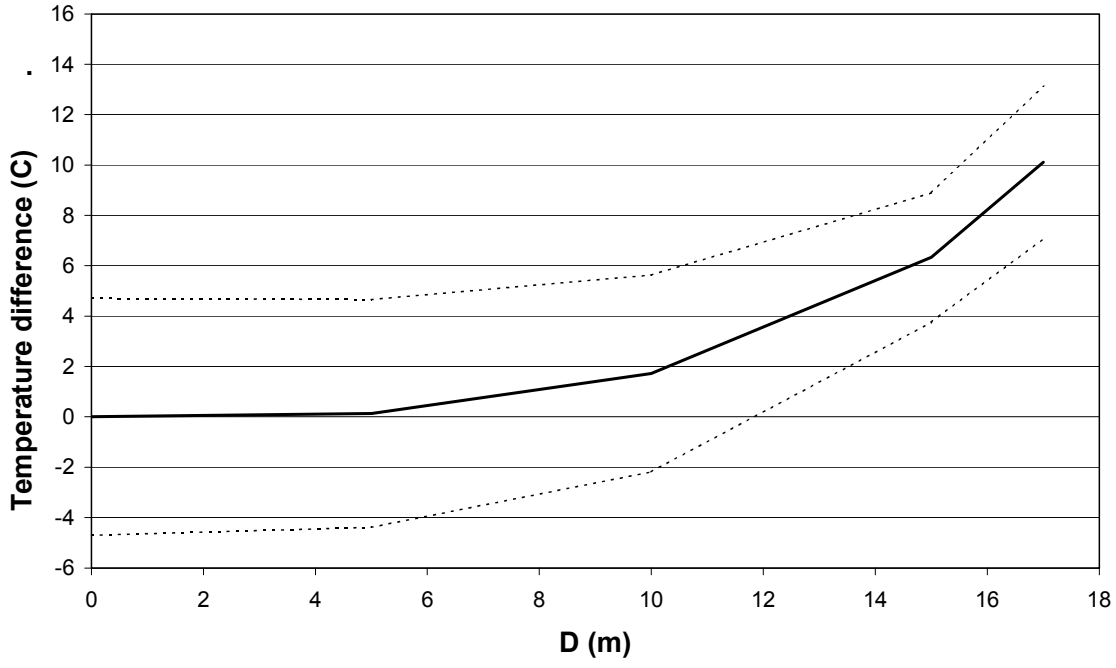

Figure A2-7. *Case C. Borehole surrounded by rock species A. Increasing peripheral fraction of species B. See Figure A2-6. The solid line shows the average value of the difference in steady-flux temperature compared to a situation where the considered calculation area consists of rock species A with homogeneous thermal conductivity of 3,4 W/m,K. The dashed lines indicate the standard deviation.*

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Claesson J, Probert T, 1996. Temperature field due to time-dependent heat sources in a large rectangular grid. I. Derivation of analytical solution. Depts.of Building Physics and Mathematical Physics, Lund University.

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