R-06-13

Thermal modelling

Preliminary site description Laxemar subarea – version 1.2

Jan Sundberg, John Wrafter, Pär-Erik Back, Märta Ländell
Geo Innova AB

February 2006

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1402-3091
SKB Rapport R-06-13

Thermal modelling

Preliminary site description Laxemar subarea – version 1.2

Jan Sundberg, John Wrafter, Pär-Erik Back, Märta Ländell
Geo Innova AB

February 2006

Summary

This report presents the thermal site descriptive model for the Laxemar subarea, version 1.2. The main objective of this report is to present the thermal modelling work where data has been identified, quality controlled, evaluated and summarised in order to make an upscaling to lithological domain level possible.

The thermal conductivity at canister scale has been modelled for five different lithological domains: RSMA (Ävrö granite), RSMBA (mixture of Ävrö granite and fine-grained dioritoid), RSMD (quartz monzodiorite), RSME (diorite/gabbro) and RSMM (mix domain with high frequency of diorite to gabbro). A base modelling approach has been used to determine the mean value of the thermal conductivity. Four alternative/complementary approaches have been used to evaluate the spatial variability of the thermal conductivity at domain level. The thermal modelling approaches are based on the lithological domain model for the Laxemar subarea, version 1.2 together with rock type models based on measured and calculated (from mineral composition) thermal conductivities. For one rock type, Ävrö granite (501044), density loggings have also been used in the domain modelling in order to evaluate the spatial variability within the Ävrö granite. This has been possible due to an established relationship between density and thermal conductivity, valid for the Ävrö granite.

Results indicate that the means of thermal conductivity for the various domains are expected to exhibit a variation from 2.45 W/(m·K) to 2.87 W/(m·K). The standard deviation varies according to the scale considered, and for the 0. 8 m scale it is expected to range from 0.17 to 0.29 W/(m·K). Estimates of lower tail percentiles for the same scale are presented for all five domains. The temperature dependence is rather small with a decrease in thermal conductivity of 1.1–5.3% per 100°C increase in temperature for the dominant rock types.

There are a number of important uncertainties associated with these results. One of the uncertainties relates to the representative scale for the canisters, although recent studies have shown that variability at scales below between 1 and 2 m are irrelevant for the temperature at the canister. Another important uncertainty is the methodological uncertainties associated with the upscaling of thermal conductivity from centimetre scale to canister scale. In addition, the representativeness of rock samples is uncertain and it is not known how large the bias, introduced by judgmental sample selection is. A potential bias in the calculated thermal conductivity values from density loggings may affect the results at domain level for domains in which Ävrö granite is a major component.

For the Laxemar model version 1.2, thermal conductivity has been estimated for two lithological domains previously described in the Simpevarp site description model version 1.2, namely domains RSMA and RSMD. For RSMA, the results from Laxemar 1.2 are similar to those from Simpevarp 1.2. For RSMD, the Laxemar data produces a somewhat higher mean thermal conductivity. Variability within domain RSMA is estimated to be similar to that predicted in Simpevarp 1.2, but for domain RSMD considerably smaller than in Simpevarp 1.2.

Mean values of heat capacity range from 2.23 to 2.29 MJ/(m^3·K) for four of the lithological domains modelled according to a Monte Carlo simulation. The standard deviation varies only slightly (0.12 to 0.13 MJ/(m^3·K)). The heat capacity exhibits large temperature dependence, approximately 25% increase per 100°C temperature increase for the three dominant rock types investigated.

The mean coefficient of thermal expansion for the three dominant rock types was determined to between $6.9 \cdot 10^{-6}$ and $8.2 \cdot 10^{-6}$ m/(m·K).

In situ temperature has been measured in five boreholes. The mean of all temperature loggings is 13.9°C at 500 m depth which compares with 14.4°C calculated from five boreholes in the Simpevarp model version 1.2. Temperature vs depth is presented in both tables and figures for each borehole. There is a variation in temperature between the boreholes at a specified depth.

Different loggings in the same borehole give slightly different results, indicating that there are potential errors. Possible sources of uncertainty in the temperature logging results include calibration error, timing of the logging after drilling, water movements along the boreholes and measured inclination of the boreholes.

Sammanfattning

Föreliggande rapport presenterar den termiska platsbeskrivande modellen för Laxemarsområdet, version 1.2. Syftet med denna rapport är att presentera det termiska modelleringsarbetet där data har identifierats, kvalitetssäkrats, utvärderats och sammanfattats för att möjliggöra en uppskalning till litologisk domännivå.

Den termiska konduktiviteten i kapselskala har modellerats för fem olika litologiska domäner (RSMA (Ävrö granit), RSMBA (blandning av Ävrögranit och finkornig dioritoid), RSMD (kvartsmonzodiorit), RSME (diorit/gabbro) och RSMM (blanddomän med stor förekomst av diorit och gabbro)). Ett grundläggande angreppssätt för den termiska modelleringen har använts för bestämning av den termiska konduktivitetens medelvärde. Fyra alternativa/kompletterande angreppssätt har använts för att utvärdera den termiska konduktivitetens spatiala variation på domännivå. Den termiska modelleringens olika angreppssätt baseras på den litologiska domänmodellen för Laxemarsområdet version 1.2 tillsammans med bergartsmodeller upprättade med utgångspunkt ifrån mätningar och beräkningar (utifrån mineralsammansättning) av den termiska konduktiviteten. För en bergart, Ävrö granit (501044), har densitetsloggningar uppmätta inom den specifika bergarten också använts i domänmodelleringen för att uppskatta den spatiala variationen inom just Ävrö graniten. Detta har varit möjligt på grund av ett presenterat samband mellan densitet och termisk konduktivitet gällande för Ävrö granit.

Resultaten indikerar att medelvärdet för den termiska konduktiviteten förväntas variera mellan 2,45 W/(m·K) till 2,87 W/(m·K) mellan de olika domänerna. Standardavvikelsen varierar beroende på vilken skala som bedöms, för kapselskalan (0,8 m) förväntas den variera mellan 0,17 och 0,29 W/(m·K). En skattning av låga percentiler presenteras i samma skala för alla fem domänerna. Temperaturberoendet är relativt litet med en minskning i termisk konduktivitet på 1,1–5,3 % per 100°C temperaturökning för de dominerande bergarterna.

Det finns ett antal viktiga osäkerheter associerade med dessa resultat. En av osäkerheterna berör den representativa skalan för kapseln, men nyare undersökningar har visat att variabiliteten i skalor under ca 1–2 m inte är relevanta för temperaturer på kapseln. Ytterligare en viktig osäkerhet är de metodrelaterade osäkerheterna i samband med uppskalningen av den termiska konduktiviteten från centimeter – till kapselskala. Till detta skall även läggas osäkerheten i representativitet för bergartsproverna där det ännu inte är klargjort hur stor avvikelsen är på grund av metodiken för val av prover. Ett eventuellt systematiskt fel i termisk konduktivitet beräknad från loggad densitet, kan påverka resultaten på domännivå för domäner med stort innehåll av Ävrögranit.

För Laxemar modellversion 1.2 har termisk konduktivitet uppskattats för två litologiska domäner som även beskrevs i Simpevarp modellversion 1.2, nämligen domän RSMA och RSMD. Jämförelse mellan resultat från de båda modellversionerna visar likvärdig termisk konduktivitet för domän RSMA, medan medelvärdet är något högre (3 %) för domän RSMD i modellrapport Laxemar 1.2 än i Simpevarp 1.2. Likaledes uppskattas variationen vara lika för domän RSMA i de båda modellversionerna, medan den är mindre för RSMD i Laxemar 1.2 jämfört med Simpevarp 1.2.

Medelvärden för värmekapacitet varierar från 2,23 till 2,29 MJ/(m^3·K) för fyra av de litologiska domänerna, modellerade enligt Monte Carlo simulering. Standardavvikelsen varierar endast obetydligt (0,12–0,13 MJ/(m^3·K)). Värmekapaciteten uppvisar stort temperaturberoende, ungefär 25 % ökning per 100°C temperaturökning, för de tre dominerande bergarterna som undersökts.

Medelvärden för längdutvidgningskoefficienten bestämdes till 6,9–8,2·10^{-6} m/(m·K) för de tre dominerande bergarterna.

In situ temperatur har uppmätts i fem borrhål. Medelvärdet för samtliga temperaturloggningar är 13,9 °C vid 500 m djup jämfört med 14.4 °C beräknat för fem borrhål i Simpevarp modellversion 1.2. Temperatur relativt djup presenteras både i tabellform och i figurer för respektive borrhål. Det finns en variation i temperatur mellan de olika borrhålen för ett specifikt djup.

Olika temperaturloggningar i samma borrhål ger något skilda resultat vilket indikerar potentiella fel. Möjliga källor till osäkerheter i temperaturloggningsresultaten innefattar kalibreringsfel för mätinstrumentet, tiden för loggning relativt borrningsaktiviteten, vattenrörelser längs borrhålet och uppmätt inklination i borrhålet.

Contents

1 Introduction

The Swedish Nuclear Fuel and Waste Management Co (SKB) is responsible for the handling and final disposal of the nuclear waste produced in Sweden. Site investigations have started during 2002. The site investigations are carried out in different stages and shall provide the knowledge required to evaluate the suitability of investigated sites for a deep repository.

The interpretation of the measured data is made in terms of a site descriptive model covering geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties of the rock and surface ecosystems. The site descriptive model is the foundation for the understanding of investigated data and a base for planning of the repository design and for studies of constructability, environmental impact and safety assessment. A strategy for the thermal modelling is presented in /Sundberg 2003a/.

This report presents the thermal site descriptive model for the Laxemar subarea, version 1.2. Parallel to this modelling, a study on uncertainties, scale factors and modelling methodology has been ongoing for the prototype repository at the Äspö HRL /Sundberg et al. 2005a/. The experiences from this parallel study have been partially implemented in the present modelling report.

2 Objective and scope

The purpose of this document is to present the thermal modelling work for the Laxemar site descriptive model version 1.2. Primary data originate from the work in connection with Laxemar site descriptive model version 1.2, previous work at Äspö HRL and the Simpevarp site descriptive model versions 1.1 and 1.2. The lithological domain model for Laxemar /SKB 2006/ forms the geometric base for modelling of thermal properties. Data has been identified, quality controlled, evaluated and summarised in order to make the upscaling possible to domain level.

The thermal model of the bedrock describes thermal properties at lithological domain level which is of importance since the thermal properties of the rock mass affects the possible distance, both between canisters and deposition tunnels, and therefore puts requirements on the necessary repository volume. Of particular interest is the thermal conductivity since it directly influences the design of a repository. Measurements of thermal properties are performed at cm scale but values are requested in the canister scale and therefore the spatial variability is required to be considered. Due to this, the thermal modelling includes elements of upscaling of thermal properties which is further described in /Sundberg et al. 2005a/. The work has been performed according to a strategy presented in /Sundberg 2003a/.

3 State of knowledge at the previous model version

There is no previous model version specifically devoted to the Laxemar subarea. The Simpevarp site descriptive model version 1.2 describes the thermal properties of the adjacent Simpevarp subarea, and in doing so incorporates a limited amount of data from the Laxemar subarea. In SDM Simpevarp 1.2 /SKB 2005/, thermal properties were reported for four lithological domains, two of which are also present in the Laxemar subarea. Results indicated that the mean thermal conductivities for the different domains exhibit only a small variation, from 2.62 to 2.80 W/(m·K). Standard deviations vary according to the scale considered and for the canister scale were expected to range from 0.20 to 0.28 W/(m·K). A small temperature dependence was detected in thermal conductivity for dominant rock types. A decrease of 1.1 to 3.4% per 100°C increase in temperature was found.

The main uncertainties of the thermal modelling in Simpevarp version 1.2 were considered to be the choice of the representative scale for the canister, the methodological uncertainties associated with the upscaling of thermal conductivity from cm-scale to canister scale, the representativeness of rock samples, and the representativeness of the boreholes for the domains.

Modelling of heat capacity at domain level for the four lithological domains according to a Monte Carlo simulation gave mean values of the heat capacity ranging from 2.23 to 2.25 MJ/(m^3K) and standard deviations ranging from 0.06 to 0.12 MJ/(m^3K). The heat capacity exhibits large temperature dependence, from 25% to 32% increase per 100°C temperature increase.

The coefficient of thermal expansion was determined to 6.0–8.0E–6 m/(m·K) for the three dominant rock types.

The mean of all temperature loggings is 14.4°C at 500 m depth, but the results were associated with potential errors resulting presumably from errors associated with the logging method, as well as timing of the logging after drilling.

Much of the data from Simpevarp 1.2 is employed here to characterise the thermal properties of the rock types present in the Laxemar subarea. Together with additional data from Laxemar, both direct measurements and borehole logging, an improved representation of the thermal properties at domain level has been achieved.

4 Evaluation of primary data

The evaluation of primary data includes analyses of measurements of thermal conductivity, heat capacity, temperature dependence of thermal properties, coefficient of thermal expansion and in situ temperatures. It also includes calculations of thermal conductivity from mineral composition and establishment of rock type distributions (PDF) of thermal conductivity. The spatial variation in thermal conductivity is also investigated by using density loggings.

4.1 Summary of used data

Table 4-1 summarises the available data on thermal properties used in the evaluation. A translation key to names on rock types is available in Table 4-2. Depending on the objectives, the data used is derived from different geographical areas. For the purposes of domain modelling, data from the Laxemar subarea only is used. In order to create rock type models and to establish a relationship between thermal conductivity and density, data is taken from a wider area comprising the Simpevarp subarea, Äspö and Laxemar.

Table 4-1. Summary of data used in the evaluation of primary data.

Data specification	Ref	Rock type	Number of samples/ measurements	Borehole (depth)/surface
Laboratory thermal conductivity and diffusivity tests on cores from Laxemar, Simpevarp and old boreholes at Äspö HRL	IPR-99-17 R-02-27 P-04-53 P-04-54 P-04-55 P-04-270 P-04-258 P-04-267 /Sundberg et al. 2005a/	501044	71	KLX02 (314–315 m ,492–503 m, 738–741 m), KAV01 (508–509 m), KA2599G01 (4–127 m), KLX04A (308–313 m, 562–568 m, 739–747 m), KAV04A (521–522 m), Äspö prototype repository tunnel (section 3,539–3,587 m)
		501030	26	KSH01A (399–415 m, 480–496 m), KSH02 (311–323 m, 609–610 m, 791–802 m)
		501036	15	KSH01A (299–306 m, 703–713 m), KAV04A (492–496 m)
		511058	2	KA2599G01 (50–62 m)
Modal analyses	P-04-53 P-04-54 P-04-55 P-04-258 P-04-270 P-04-270 P-04-102 SICADA database, field note no 34 and 538	501044	86	KLX01, KLX02, KLX03, KLX04, KSH01A, KAV01, KAV04A, surface
		501030	31	KLX02, KSH01A , KSH02, surface

Data specification	Ref		Rock type	Number of samples/ measurements	Borehole (depth)/surface
			501036	23	KLX02, KSH01A, KSH01B, KAV04A, surface
			505102	10	KLX01, KLX02, surface
			501033	7	surface
			511058	10	KLX01, KLX02, surface
			501058	5	surface
Density logging	Results	Interpret.			
	P-03-111 P-04-280 P-04-306 P-04-202 SICADA activity ID 12924140	P-05-34 P-04-214 P-04-217	501044	26,727	KLX02 (201.5–1,004.9 m) KLX03 (101.8–999.9 m) KLX04 (101.6–990.2 m) KAV04A (101.0–1,002.2 m) KLX01 (1.0–701.6 m)
Temperature and gradient logging	Results	Interpret.			
	P-03-111 P-04-280 P-04-306 P-04-202 SICADA activity ID 3012572	P-05-34 P-04-214 P-04-217			KLX01 KLX02 KLX03 KLX04 KAV04A
Boremap logging	P-04-195, P-04-239, P-04-275, P-04-129, P-04-231, and SICADA database				KLX01, KLX02, KLX03, KLX04, KAV04A
Laboratory tests of thermal expansion	P-04-59 P-04-60 P-04-61 P-04-272 P-04-269		501044	41	KAV01 (505–509 m), KAV04A (519–522 m), KLX02 (314–322 m, 493–507 m, 736–742 m) KLX04 (306–313 m, 560–565 m, 737–739 m)
			501030	17	KSH01A (399–412 m, 480–493 m), KSH02 (312–327 m)
			501036	14	KSH01A (298–303 m, 701–714 m), KAV04A (492–495 m)

4.2 Geological introduction

The bedrock of the Laxemar area, for which the thermal site descriptive model version 1.2 has been conducted, is predominated by two rock types, namely:

- Ävrö granite
- Quartz monzodiorite

Besides the two dominant rock types, several subordinate rock types occur within the bedrock area for the thermal model. For an illustration of the rock type classification and bedrock geology, see Figure 4-1. The main difference in lithology between the Laxemar and

Simpevarp subareas concerns the importance of fine-grained dioritoid. In Simpevarp this rock type is of major importance /Nilsson et al. 2004/, while in Laxemar it is much less extensive /Wahlgren et al. 2004/.

Subsequently in this report, rock types will occasionally be identified and described by their name codes. Therefore, a translation table linking name code to rock name is given in Table 4-2.

Data from different boreholes, mainly from within the Laxemar subarea, but also one from the Simpevarp subarea, have been used and are evaluated in this report. Figure 4-1 illustrates the location of the boreholes.

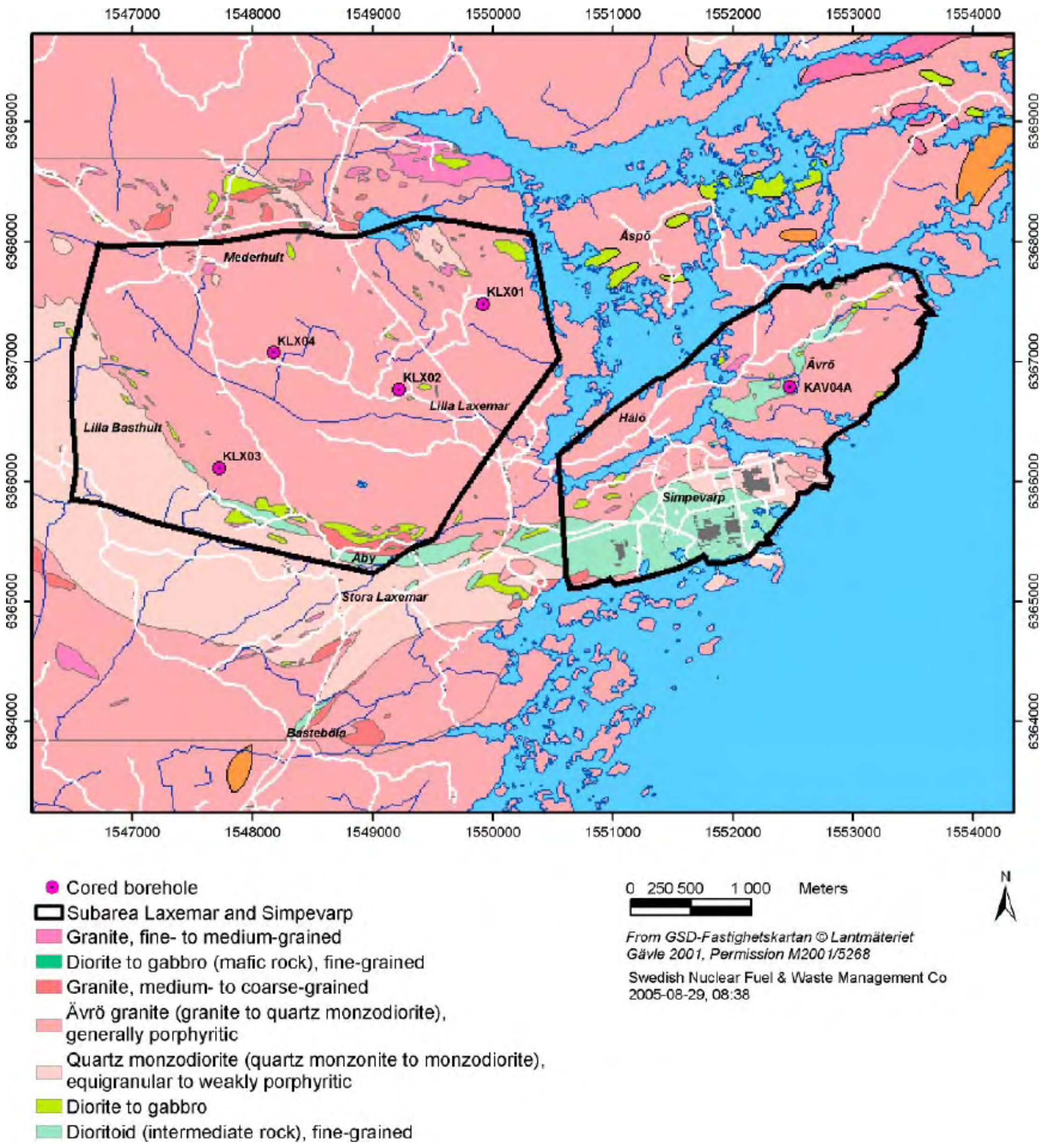

***Figure 4-1.** Bedrock geology of the Laxemar and Simpevarp subareas with the location of boreholes referred to in this report.*

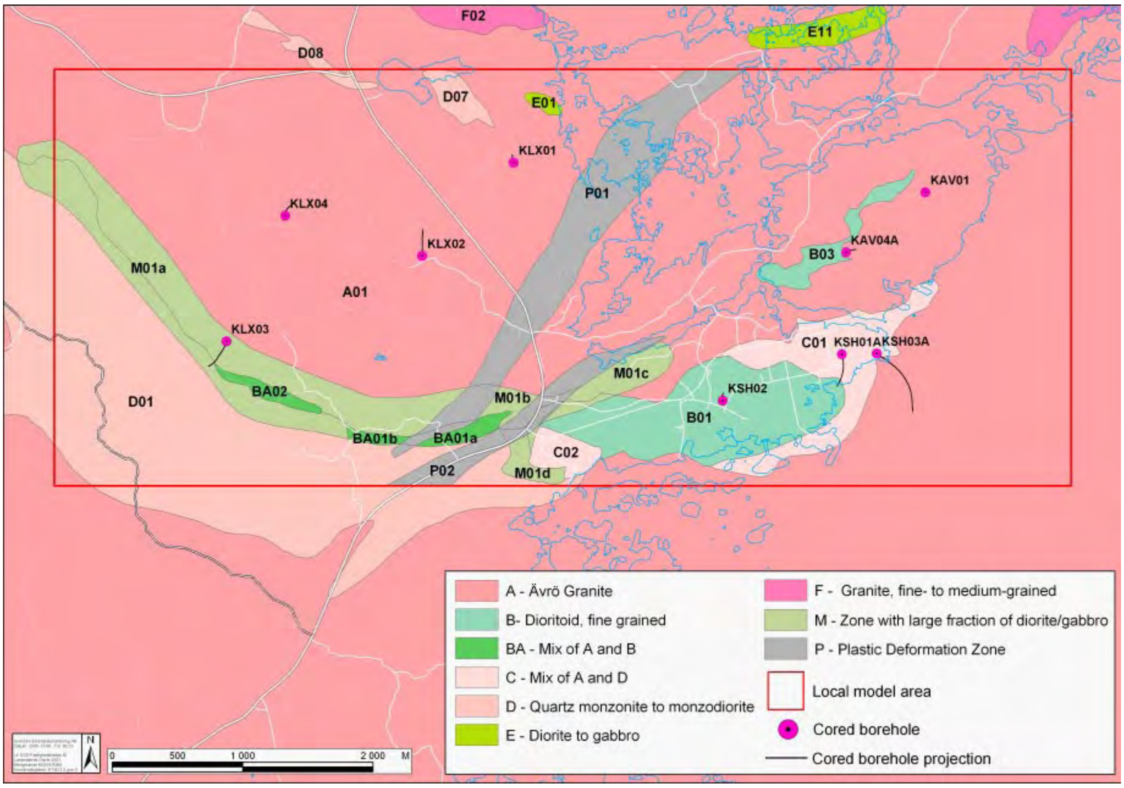

Figure 4-2. Surface view of lithological domains, including subdomains. The rectangular area includes both the Laxemar and Simpevarp subareas.

Table 4-2. Rock names and name codes.

Name code	Rock name
501044	Ävrö granite
501036	Quartz monzodiorite
501030	Fine-grained dioritoid
505102	Fine-grained diorite-gabbro
501033	Diorite/gabbro
511058	Fine-grained granite
501058	Granite

A three-dimensional lithological model comprising several rock domains has been constructed for the Laxemar subarea /SKB 2006/. Each domain may comprise one or more subdomains. Figure 4-2 shows the surface extent of the defined domains Thermal properties of five types of lithological rock domain within the Laxemar subarea, roughly the area west of the plastic deformation zone (domain P01 in Figure 4-2), will be calculated and presented within this report: domains RSMA, RSMBA, RSMD, RSMM, and RSME. Classifying rock volumes in different domains is a way of processing and simplifying rock volumes with, relatively speaking, the same key geological properties. The dominant rock type in domain RSMA is Ävrö granite, in domain RSMBA both Ävrö granite and fine-grained dioritoid, in RSMD quartz monzodiorite, and RSME diorite to gabbro. Domain RSMM includes a large fraction of diorite/gabbro in a zone comprising both Ävrö granite and Quartz monzodiorite. For a more detailed description of the rock type composition in the different lithological domains, see Table 5-4.

4.3 Thermal conductivity and diffusivity from measurements

4.3.1 Method

Laboratory measurements of the properties thermal conductivity and thermal diffusivity have been performed with the Transient Plane Source method (TPS) /Gustafsson 1991/. The TPS method can be used for measurements of thermal diffusivity and thermal conductivity of both fluids and solids, from cryogenic temperatures to approximately 250°C (if the sensor insulation is made of kapton). Measurements of thermal properties using the TPS method have been used previously by SKB /Sundberg and Gabrielsson 1999, Sundberg 2002, Sundberg et al. 2005ab/ and also within the thermal programme of the site investigations.

Prior to the measurements, the rock samples from the drill core are cut in two halves, each with a thickness of approximately 25 mm. The two intersection surfaces need to be relatively smooth in order to limit the contact resistance between the probe and the sample surface.

The principle of the TPS instrument is to place a circular probe consisting of a Ni-spiral covered by an insulating material (usually kapton, at high temperatures mica is used) between the two sample pieces. The sensor generates a heat pulse while simultaneously the heating of the specimen is recorded. The heat pulse is selected to achieve a heat increase of about 1K at the sample surfaces facing the sensor. The output power and the duration of the pulse are dependent on sample size, material properties and sensor diameter. The thermal properties can be evaluated by using the fact that the resistance for the thin Ni-spiral at any time is a function of its initial resistance, the temperature increase and the temperature coefficient for the resistivity of nickel. The measured temperatures is stored in the software and by comparing these values to a theoretical solution based on assumptions regarding a plane sensor and an infinite sample in perfect contact with the sensor surface, the thermal diffusivity and thermal conductivity can be determined. The volumetric heat capacity can thereafter be calculated.

According to the manufacturer the accuracy of the thermal conductivity measurements is ± 2%, thermal diffusivity ± 5% and specific heat ± 7% /HotDisk 2004/. This is accomplished if the sample size, sensor diameter, output of power and total time of the temperature measurement is properly selected in addition to allowing the sample reach temperature equilibrium before beginning the measuring process.

Measurements on samples from the Laxemar area have been conducted by SP (Swedish National Testing and Research Institute).

4.3.2 Compared TPS tests

As part of the quality assurance of thermal properties data, 10 samples from KSH01A comprising rock types fine-grained dioritoid and quartz monzodiorite were selected to compare TPS measurements at two different laboratories, Hot Disk AB /Dinges 2004/ and SP (Swedish National Testing and Research Institute) /Adl-Zarrabi 2004b/. The samples have been measured at three different temperatures and the results are presented in Table 4-3 and Table 4-4. In Table 4-3 the results at all three temperatures are included, while in Table 4-4 only the results at 20°C are used. A comparison of the results from the two different laboratories is shown in Figure 4-3.

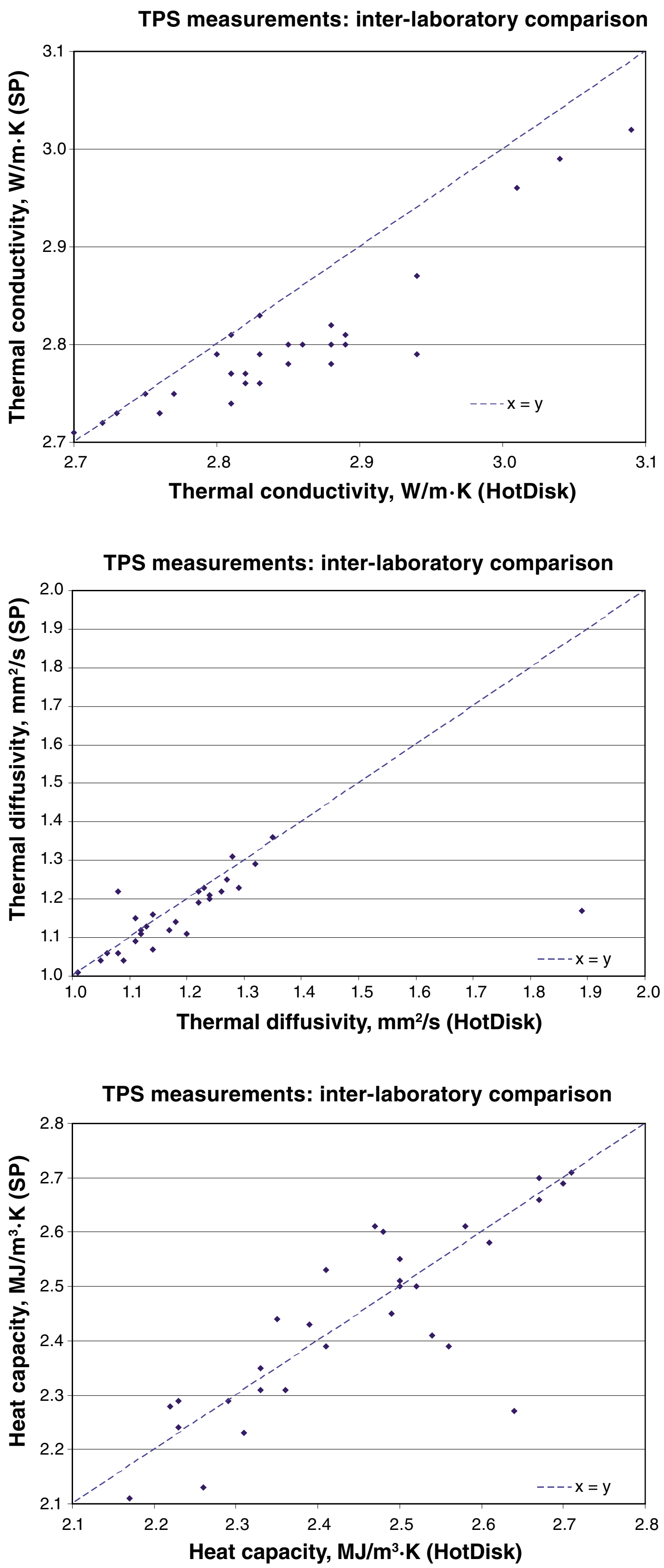

Figure 4-3. *Comparison of results for thermal conductivity, heat capacity and thermal diffusivity measured according to the TPS method. Measurements were made by both Hot Disk AB and SP (Swedish National Testing and Research Institute). Points falling on the x = y line yielded identical values in both laboratories.*

Table 4-3. Comparison of results of TPS measurements performed by two different laboratories, Hot Disk and SP, on the same samples from borehole KSH01A. Data are based on 30 measurements (10 samples, investigated at three different temperatures: 20°C, 50°C and 80°C).

	Thermal conductivity (W/(m·K))		Heat capacity (MJ/(m³·K))		Thermal diffusivity (mm²/s)[1]	
	SP	Hot Disk	SP	Hot Disk	SP	Hot Disk
Mean	2.80	2.85	2.44	2.45	1.15	1.17
Std dev	0.07	0.09	0.17	0.16	0.09	0.09
Diff (Hot Disk-SP)/SP	1.70%		0.49%		1.14%	

[1] One outlier omitted from statistical calculations.

Table 4-4. Results of TPS measurements at 20°C for 10 samples from borehole KSH01A. Measurements performed by two laboratories, Hot Disk and SP.

	Thermal conductivity (W/(m·K))		Heat capacity (MJ/(m³·K))		Thermal diffusivity (mm²/s)[1]	
	SP	Hot Disk	SP	Hot Disk	SP	Hot Disk
Mean	2.82	2.88	2.26	2.28	1.26	1.28
Std dev	0.08	0.09	0.09	0.07	0.05	0.04
Diff (Hot Disk-SP)/SP	2.31%		0.71%		1.59%	

[1] One outlier omitted from statistical calculations.

For thermal conductivity the measured difference on the same sample varies from –0.37% to 3.60% which in thermal conductivity means –0.01 W/(m·K) to 0.10 W/(m·K). A systematic bias is apparent, the SP results being on average 0.05 W/(m·K) lower than the Hot Disk results, Table 4-3. The difference in heat capacity measured for the same sample varies between –5.36% to 16.30% which expressed in heat capacity equates to –0.14 MJ/(m³·K) to 0.37 MJ/(m³·K). For a more detailed report of this inter-laboratory comparison see /Sandström 2005/.

4.3.3 Results

In Table 4-5 and Table 4-6 the results from all performed laboratory measurements of thermal conductivity and thermal diffusivity are summarised. Due to the small scale of the measurements, the variability in the results is possibly overestimated compared to a larger scale. Observe that samples from rock type Ävrö granite (501044) have been collected from the Simpevarp subarea /Adl-Zarrabi 2004abcd /, the Laxemar subarea /Adl-Zarrabi 2004ef/ and the Äspö HRL /Sundberg and Gabrielsson 1999, Sundberg 2002, Sundberg et al. 2005a/. Samples from rock type fine-grained dioritoid (501030) and quartz monzodiorite (501036), with the exception of two samples of 501036 from Äspö, all come from the Simpevarp subarea /Adl-Zarrabi 2004abcd/.

The data from Äspö HRL and boreholes KSH01A, KSH02 and KAV01 in the Simpevarp subarea are described in more detail in /Sundberg et al. 2005b/. Recently acquired data (39 measurements) for boreholes KLX02, KLX04 and KAV04A are presented in Figure 4-4. All of the samples from these boreholes are located in spatial proximity to other samples with approximately 2–5 samples in each group, which is apparent from Figure 4-4. The majority of samples selected for measurement are from rock that is either unaltered or has been judged to have only faint alteration. Rocks with weak, medium or strong alteration, which comprise about 10–15% of the boreholes /SKB 2006/, have not been sampled. This may introduce a bias to the results since many of the observed alteration products, for example chlorite, have higher thermal conductivities than their parent minerals. For a more in-depth discussion see Section 4.4.

Table 4-7 presents the data according to geographical location. From Table 4-7 it would appear that the mean thermal conductivity for Ävrö granite is higher for Laxemar and Simpevarp samples than for the Äspö samples. A two-sample t-test confirms that the difference between TPS-values in the Laxemar subarea and Simpevarp subarea is not significant at the 5% level. These observations, however, may simply be an artefact of sampling. Thermal conductivities modelled from density logging indicate that low values occur even in the Laxemar area.

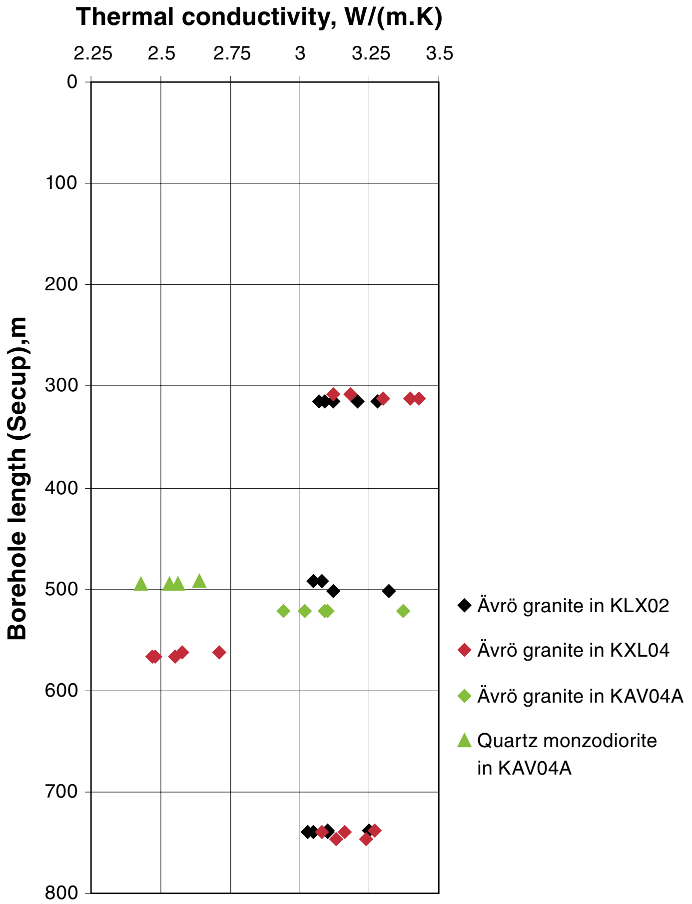

Figure 4-4. *Location (borehole length) and thermal conductivity of samples measured with the TPS method differentiated on the basis of rock name and borehole.*

Table 4-5. Measured thermal conductivity (W/(m·K)) of samples using the TPS method. Samples are from boreholes KAV01, KAV04A, KSH01A, and KSH02 (Simpevarp subarea), boreholes KLX02 and KLX04 (Laxemar subarea) together with borehole KA2599G01 (Äspö HRL) and the prototype repository tunnel (Äspö HRL).

Rock name	Name code	Sample location	Mean	Std dev	Max	Min	Number of samples
Fine-grained dioritoid	501030	Boreholes KSH01A and KSH02.	2.79	0.16	3.16	2.51	26
Quartz monzodiorite	501036	Boreholes KSH01A, KAV04A.	2.74	0.16	2.95	2.43	15
Ävrö granite	501044	Boreholes KAV04A, KLX02 KLX04, KAV01, KA2599G01, Äspö HRL prototype tunnel.	2.90	0.35	3.76	2.16	71
Fine-grained granite	511058	Borehole KA2599G01	3.63	0.07	3.68	3.58	2

Table 4-6. Measured thermal diffusivity (mm^2/s) of samples using the TPS method. Samples are from boreholes KAV01, KAV04A, KSH01A, and KSH02 (Simpevarp subarea), and boreholes KLX02 and KLX04 (Laxemar subarea).

Rock name	Name code	Sample location	Mean	Std dev	Number of samples
Fine-grained dioritoid	501030	Boreholes KSH01A, KSH02.	1.28	0.16	26
Quartz monzodiorite	501036	Boreholes KSH01A, KAV04A.	1.21	0.11	15
Ävrö granite	501044	Boreholes KAV04A, KLX02, KLX04, KAV01.	1.38	0.14	39

Table 4-7. Summary of TPS measurements for various rock units according to geographical location.

		Laxemar subarea	Simpevarp subarea	Äspö
Ävrö granite	Mean	3.07	3.18	2.55
501044	Std dev	0.26	0.23	0.29
	No of samples	*29*	*10*	*32*
Quartz monzodiorite	Mean		2.74	
501036	Std dev		0.16	
	No of samples		15	
Fine-grained dioritoid	Mean		2.79	
501030	Std dev		0.16	
	No of samples		26	
Fine-grained granite	Mean			3.63
511058	Std dev			0.07
	No of samples			2

4.3.4 Temperature dependence

The temperature dependence of thermal conductivity has been investigated by laboratory measurements, for the two rock types fine-grained dioritoid (501030) and quartz monzodiorite (501036), at three different temperatures (20, 50 and 80°C) /Adl-Zarrabi 2004ab/, and for rock type Ävrö granite (501044), the thermal conductivity has been measured on four samples at four different temperatures (25, 40, 60 and 80°C) /Sundberg 2002/, and on a further 9 samples at three different temperatures (20, 50 and 80°C) /Adl-Zarrabi 2004de/.

Results for fine-grained dioritoid (501030) and quartz monzodiorite (501036), as well as four sample of Ävrö granite are presented in /Sundberg et al. 2005b/. Figure 4-5 displays the results for additional Ävrö granite samples while Table 4-8 summarises the temperature dependence of thermal conductivity for the three separate rock types. From Figure 4-5 it would appear that temperature dependence is greater for samples having higher thermal conductivities than it is for samples with low conductivity.

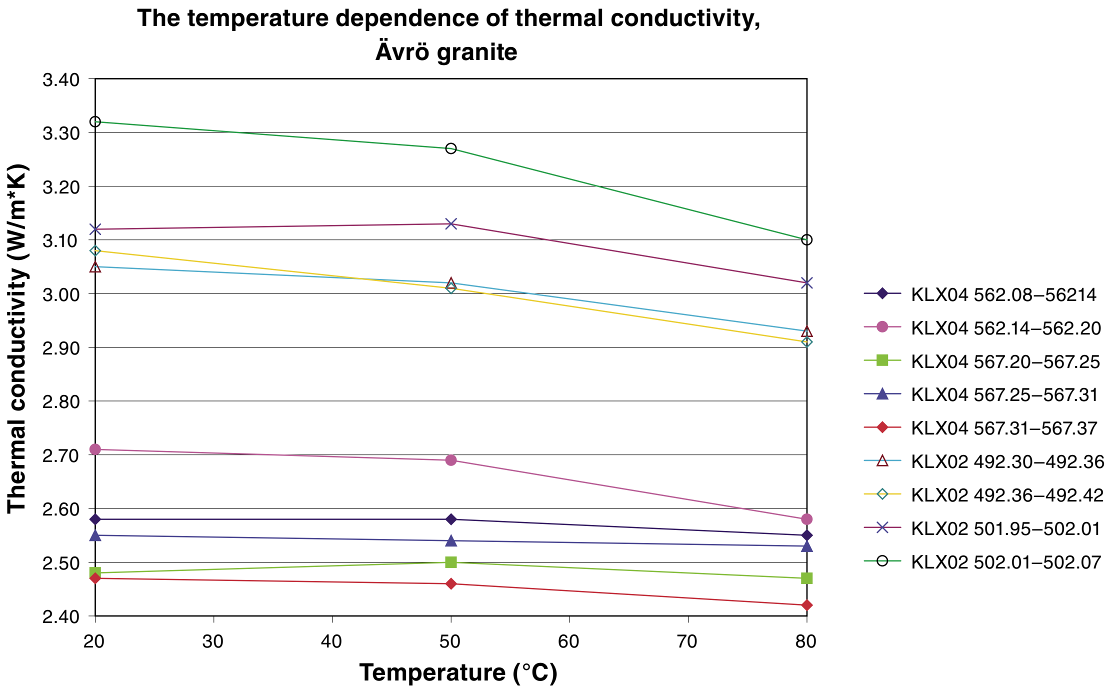

Figure 4-5. *Temperature dependence of thermal conductivity, rock type Ävrö granite (501044).*

Table 4-8. Measured temperature dependence of thermal conductivity (per 100°C temperature increase) for different rock types from boreholes KSH01A, KSH02 (Simpevarp subarea), KA2599G01 (Äspö HRL), and KLX02 and KLX04 (Laxemar subarea). Mean value of temperature dependence calculated by linear regression.

Rock name	Name code	Sample location	Mean	Std dev	Number of samples
Fine-grained dioritoid	501030	Boreholes KSH01A and KSH02.	–3.4%	1.6%	11
Quartz monzodiorite	501036	Borehole KSH01A.	–1.1%	1.1%	5
Ävrö granite	501044	Borehole KA2599G01.	–2.3%	3.7%	4
Ävrö granite	501044	Boreholes KLX02 and KLX04.	–5.3%	3.7%	9

4.4 Thermal conductivity from mineral composition

4.4.1 Method

Thermal conductivity of rock samples can be calculated with the SCA method (Self Consistent Approximation) using mineral compositions from modal analyses and reference values of the thermal conductivity of different minerals /Dagan 1979, Sundberg 1988, Sundberg 2003a/. The calculations are performed at the millimetre scale. Although calculated values have earlier been shown to be in good agreement with measured values /Sundberg 1988, Sundberg 2002/, more recent studies in the Simpevarp subarea /Sundberg et al. 2005b/ reveal significant discrepancies.

The following data were used for calculations with the SCA method. Previously processed data comprise:

- Modal analyses from the SICADA database performed in conjunction to Simpevarp site descriptive model version 1.1, reclassified rock types (62 samples) /Wahlgren 2004/.
- Modal analyses in conjunction with measurements of thermal properties on samples from boreholes KAV01, KSH01A and KSH02 (a total of 16 samples, of which six have been recalculated – not in SICADA as of 15 October, 2005 – and are included in the data analysis) /Wahlgren 2004/.
- Modal analyses on samples from boreholes KLX01 and KLX02 (39 samples).
- Data from Äspö has been excluded since SCA calculations were performed in such a way that they are not directly comparable with the rest of the data set.

New data comprises:

- Modal analyses on samples proximal to samples on which thermal properties were measured; from boreholes KLX02 (6 samples), KLX04 (6 samples) and KAV04A (5 samples) /Adl-Zarrabi 2004def/.
- Modal analyses on 5 samples from borehole KLX03, in addition to 51 surface samples, the majority from the Laxemar subarea, and collected as part of the geological programme (SICADA database, Field note no 34 and no 538). Of the surface samples, a total of eight samples are from the area west of the Laxemar subarea (6 of 501044; 1 each of 501036 and 501058). All but one has been omitted. Because of the lack of data for rock type 501058, the sample from this rock type is included in the summary table below.

For this recently acquired data, mineral percentages were normalised to 100% after subtracting the amount of unidentified minerals. Unidentified minerals were absent in most samples, and in only one case exceeded 1%.

Reference values of thermal conductivity for different minerals have been taken from /Horai 1971, Horai and Baldridge 1972/. In Table 4-9 the thermal conductivities of minerals used are presented. The values are identical to those used in Simpevarp site descriptive model version 1.2. The thermal conductivity of plagioclase, olivine and pyroxene depends on the chemical composition and may therefore vary within a certain interval. Because of this, these minerals are marked with red in Table 4-9. For minerals marked in yellow no reference values of the thermal conductivity have been found and an estimated value of 3.00 W/(m·K) have been used. Generally speaking, these minerals make up only a small proportion of the mineral composition and therefore have an insignificant influence on the

Table 4-9. Summary of used thermal conductivities (W/(m·K)) of minerals /Horai 1971, Horai and Baldridge 1972/.

Mineral	Laxemar 1.2
Allanite	3.00
Amphibole	3.39
Apatite	1.38
Biotite	2.02
Calcite	3.59
Chlorite	5.15
Clinopyroxene	3.20
Epidote	2.83
Fluorite	9.51
Hornblend	2.81
K-feldspar	2.29
Muscovite	2.32
Olivine	4.57
Opaque	3.00
Orthopyroxene	3.20
Plagioclase	1.70
Prehnite	3.58
Pumpellyite	3.00
Pyroxene	3.20
Quartz	7.69
Titanite	2.34
Zircon	4.54
Zoisite	2.15

Yellow: data missing, estimated values.
Red: unknown chemical composition of the mineral.

thermal conductivity of the rock. The thermal conductivity value chosen for K-feldspar is an average value (2.29 W/(m·K)) for the different forms of this mineral. A value based on the orthoclase mineral (2.51 W/(m·K) would have been more correct, and will be adopted in future calculations.

The thermal conductivity of the plagioclase mineral is dependent on the anorthite content. This has been taken into account when calculating the thermal conductivity of rock samples. The anorthite content is in turn controlled by the nature of the igneous rock. Typical plagioclase compositions in plutonic rocks which are common in the Simpevarp-Laxemar are granodiorite (An 25), quartz monzodiorite (An 35), quartz diorite (An 40) and Gabbro (> An 50). In Figure 4-6 the relationship between thermal conductivity and the anorthite content of plagioclase is presented with a polynomial regression line. For the Simpevarp and Laxemar subareas the anorthite content of dominant rock types has been assumed to be 30% /Wahlgren 2004/. When this anorthite content is applied to the regression ($y = 0.0002x^2+0.0246x+2.2563$) the thermal conductivity of plagioclase within the Simpevarp subarea is set to 1.70 W/(m·K). Varying the anorthite content up or down by 10% for a rock with 50% plagioclase would have a maximum effect in the order of ± 0.1 W/(m·K) on the calculated value of thermal conductivity for the rock sample. In cases where, due to alteration, plagioclase has a more albite composition the uncertainties associated with the calculations would be greater.

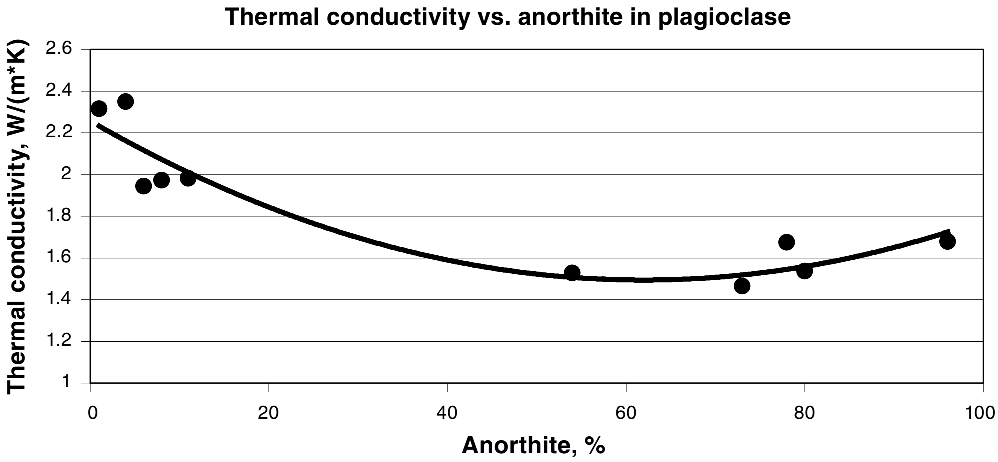

Figure 4-6. *Thermal conductivity for plagioclase versus anorthite content. Polynomial regression with equation* $y = 0.0002x^2+0.0246x+2.2563$ *and* $R^2 = 0.8845$.

4.4.2 Results

The results of the SCA calculations from both Simpevarp and Laxemar subareas are presented in Table 4-10, subdivided according to rock type.

SCA calculations from Laxemar subarea and Simpevarp subarea are compared in Table 4-11.

One sample from borehole KLX02 (secup 1,040.45 m) incorrectly assigned to Ävrö granite (in report S1.2) due to an error in linking to rock type has in this report been correctly assigned to fine-grained granite. Another sample from KLX02 assigned to rock type fine-grained dioritoid has, after a check of its mineralogy, been identified as a granite rock. The sample from borehole length 807.8 m (secup) consists of 30% quartz and 40% K-feldspar. No account of this has been taken in the results above but omitting the sample would reduce the mean thermal conductivity for fine-grained dioritoid in the Laxemar subarea.

A two-sample t-test was performed on the data for the Ävrö granite, quartz monzodiorite, fine-grained dioritoid and fine-grained granite. For Ävrö granite the mean SCA-value for the Laxemar subarea cannot be shown to be significantly different than the mean for the Simpevarp subarea at the 5% significance level. For quartz monzodiorite the means are identical. A similar test on fine-grained dioritoid does not reveal a statistically significant difference, despite the disparity in the calculated means. This is due to the limited number of samples (four) from the Laxemar area.

In general, the results based on the entire data set (i.e. from both the Laxemar and Simpevarp subareas) are not notably different to those presented in the Simpevarp site descriptive model, version 1.2.

Table 4-10. Thermal conductivity (W/(m·K)) of samples from different rock types, calculated from the mineralogical compositions (SCA method).

Rock name	Name code	Mean	Std dev	Number of samples
Fine-grained dioritoid	501030	2.43	0.33	31
Quartz monzodiorite	501036	2.41	0.14	23
Ävrö granite	501044	2.69	0.29	86
Fine-grained diorite-gabbro	505102	2.57	0.23	10
Diorite/gabbro	501033	2.41	0.22	7
Fine-grained granite	511058	3.27	0.31	10
Granite	501058	2.97	0.59	5[1]

[1] One sample taken from outside (west of) the Laxemar subarea.

Table 4-11. Summary of SCA calculations for various rock units according to geographical location.

		Laxemar subarea	Simpevarp subarea
Ävrö granite	Mean	2.71	2.62
501044	Std dev	0.31	0.23
	No of samples	*66*	*20*
Quartz monzodiorite	Mean	2.41	2.41
501036	Std dev	0.12	0.18
	No of samples	*13*	*10*
Fine-grained dioritoid	Mean	2.95	2.35
501030	Std dev	0.49	0.22
	No of samples	*4*	*27*
Fine-grained granite	Mean	3.21	3.36
511058	Std dev	0.36	0.22
	No of samples	*6*	*4*
Fine-grained diorite-gabbro	Mean	2.62	2.45
505102	Std dev	0.25	0.14
	No of samples	*7*	*3*
Diorite/gabbro	Mean	2.47	2.37
501033	Std dev	0.32	0.15
	No of samples	*3*	*4*
Granite	Mean	2.94	2.59
501058	Std dev	0.09	0.65
	No of samples	*2*	*2*

4.4.3 Geographic variation in thermal conductivity for Ävrö granite

The SCA values for Ävrö granite include samples collected from the surface at 31 localities within the Laxemar subarea. The results are presented in Figure 4-7. High thermal conductivity values (mode 3.0 W/(m·K)) occur more commonly in the central parts of Laxemar, whereas lower values (mode = 2.5 W/(m·K)) predominate in southern and north-eastern areas. Data for quartz monzodiorite (501036) are included for comparison purposes.

The observed pattern of high and low thermal conductivities within the Ävrö granite mirror the compositional variation observed in thin section analysis of this rock type /SKB 2006/. Quartz-rich varieties of Ävrö granite predominate in the central parts of the Laxemar subarea, whereas quartz-poor varieties occur predominantly along the southern flank close to the contact with quartz monzodiorite. The geological observations are supported by results from gamma-ray spectrometry data from helicopter-borne surveys /Triumf et al. 2003/ and on-ground surveys /Mattsson et al. 2004/, both of which indicate a rather inhomogeneous composition within Ävrö granite.

Thermal conductivity of surface samples calculated by the SCA method

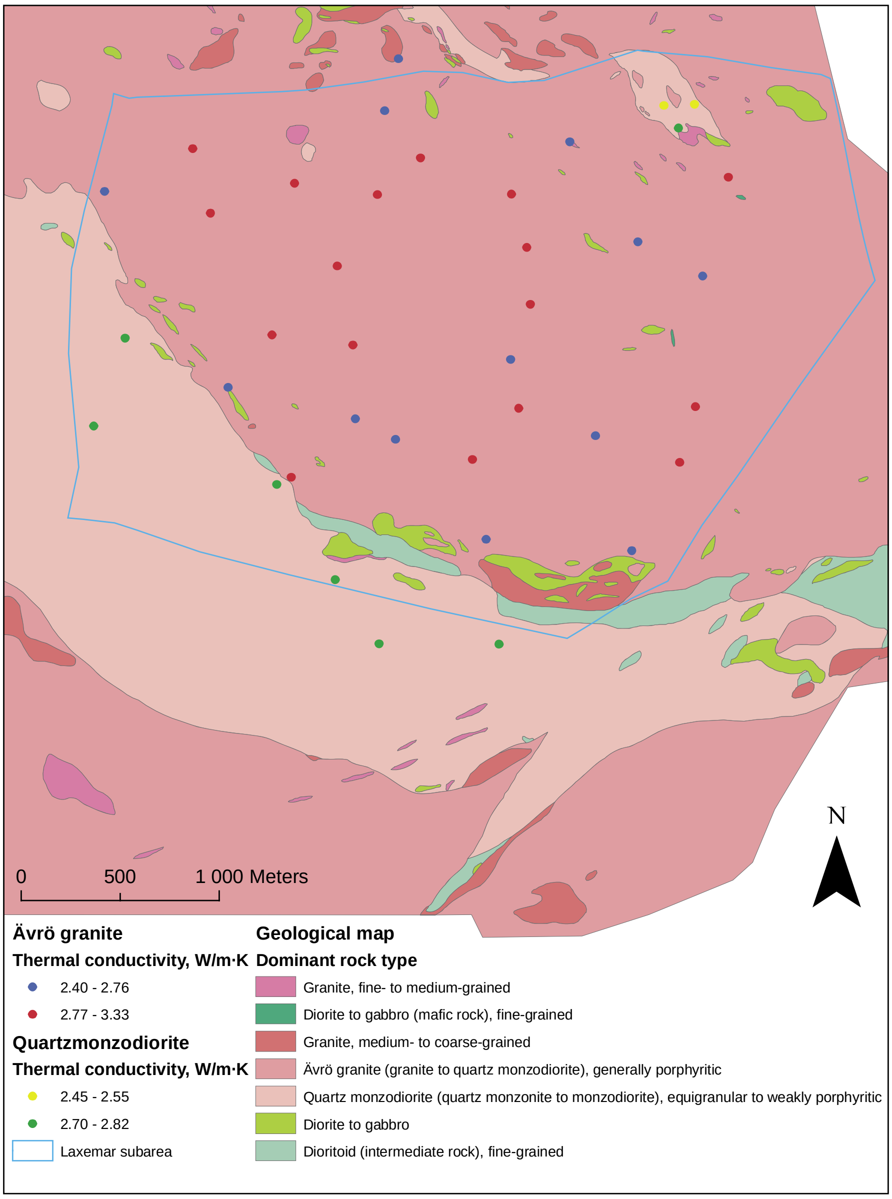

***Figure 4-7.** Thermal conductivity calculated from modal analysis (SCA method) for surface samples of Ävrö granite and, for comparison, quartz monzodiorite.*

4.4.4 Evaluation of SCA results: comparsion with measurements

In the site descriptive model Simpevarp version 1.2 it was found that calculated thermal conductivities using the SCA method were generally lower than thermal conductivities measured by the TPS method. Results from point-counting of fourteen new samples reinforce this pattern.

Alteration of some minerals, in particular plagioclase and biotite, has been observed in both the Simpevarp /SKB 2005/ and Laxemar subareas /SKB 2006/. In thermal modelling for Simpevarp 1.2, it was shown that when alteration was taken into consideration in the case of six samples (five of rock type fine-grained dioritoid (501030) and one for quartz monzodiorite (501036)), the estimated thermal conductivities were higher, by 0.23 W/(m·K) on average. The partial alteration of plagioclase to sericite and biotite to chlorite has the effect of increasing the conductive properties of rocks. Unfortunately, information regarding alteration is not available for the remaining samples analysed in conjunction with the thermal property measurements. Therefore, no quantitative evaluation can be made of the effect of alteration products on the calculated SCA values for these samples.

The degree of sericitisation of plagioclase varies from one sample to another but some degree of sericitisation is nearly always present /SKB 2006/. Even apparently unaltered rock may display sericitisation (or other alteration) to an extent which may still affect the outcome of the SCA determinations.

In Table 4-12 and Table 4-13, thermal conductivity values calculated using the SCA method are compared with measured values of proximal samples. The rock types for which data are available are as follows:

- Fine-grained dioritoid (501030) – 5 samples.
- Quartz monzodiorite (501036) – 3 samples.
- Ävrö granite (501044) – 18 measurements from Äspö HRL in addition to 12 samples from boreholes KLX02, KLX04 and KAV04A.

The rock types of the Äspö samples have been reclassified from Äspö to Simpevarp nomenclature /Wahlgren 2004/. The results from these measurements are presented in the Simpevarp thermal site descriptive model 1.2. In Table 4-12 a comparison of TPS and SCA data for recently acquired analyses is presented. Table 4-13 summarises all the available data. The results indicate a potential bias in the SCA calculations for all rock types (systematic deviations between measurements and calculations).

The difference between measured (TPS) and calculated (SCA) values of thermal conductivity for Ävrö granite is greater for samples from Laxemar and Simpevarp compared to the Äspö samples reported previously /Sundberg et al. 2005a/. This may be partly an effect of differences between the SCA calculation method used in both cases.

The data was investigated to see if the degree to which the SCA method underestimates thermal conductivity bears any relationship to the "true" (measured) thermal conductivity. Based on 15 samples (12 Ävrö granite and 3 quartz monzodiorite), no trend could be discerned (Figure 4-8). Neither is there any relationship between TPS-SCA discrepancies and mineralogy, for example percentage quartz or plagioclase.

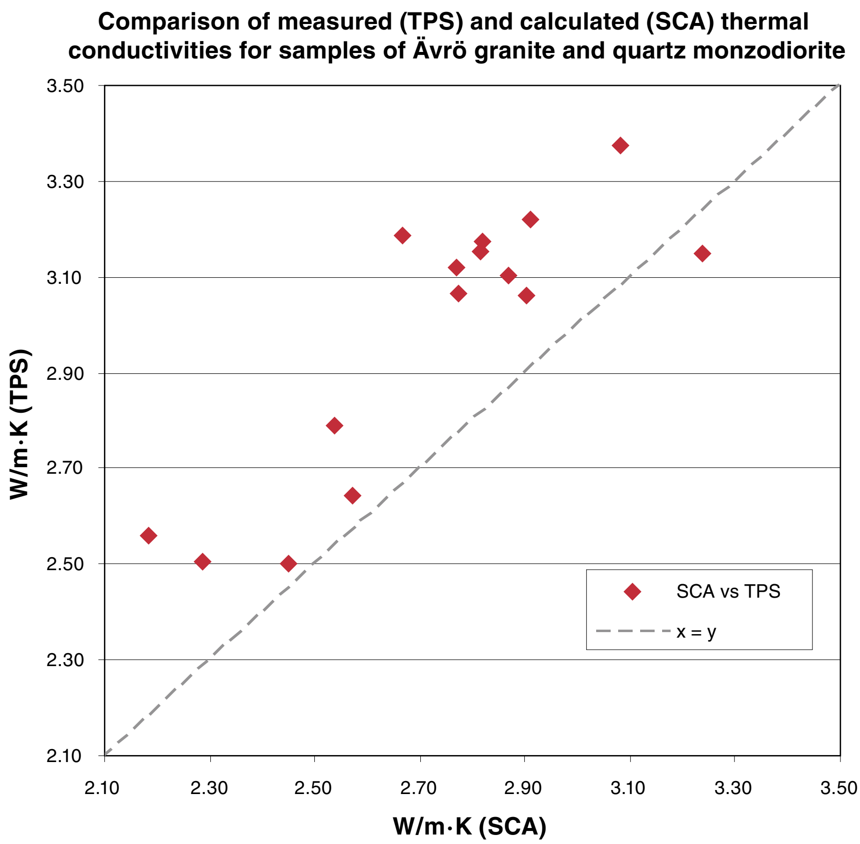

Figure 4-8. TPS versus SCA data for the "same" samples.

Table 4-12. Specification of samples included in the comparison of thermal conductivity (W/(m·K)) calculated from mineral composition (SCA) and measured with TPS method.

Borehole/ sample ID	Secup (m)	Name code	SCA	No of samples	TPS	No of samples	Diff (SCA-TPS)/TPS (%)
KLX02	314.63	501044	2.81	1	3.15	5	–10.78%
KLX02	492.28	501044	2.77	1	3.07	2	–9.54%
KLX02	502.19	501044	2.91	1	3.22	2	–9.60%
KLX02	738.34	501044	2.82	1	3.18	2	–11.18%
KLX02	740.26	501044	2.90	1	3.06	3	–5.09%
KLX04	308.11	501044	3.24	1	3.15	2	2.82%
KLX04	312.31	501044	3.08	1	3.38	3	–8.73%
KLX04	562.05	501044	2.57	1	2.65	2	–2.76%
KLX04	567.18	501044	2.45	1	2.50	3	–2.00%
KLX04	739.45	501044	2.77	1	3.12	2	–11.29%
KLX04	746.36	501044	2.67	1	3.19	2	–16.24%
KAV04A	494.21	501036	2.18	1	2.56	1	–14.66%
KAV04A	494.91	501036	2.29	1	2.51	3	–8.72%
KAV04A	521.42	501044					
KAV04A	521.87	501044	2.87	2	3.10	5	–7.65%

Table 4-13. Comparison of thermal conductivity of different rock types calculated from mineralogical compositions by the SCA method and measured with the TPS method.

Method	Fine-grained dioritoid (501030) 5 samples Mean λ, (W/(m·K))	Quartz monzodiorite (501036) 3 samples Mean λ, (W/(m·K))	Ävrö granite 18 samples (Äspö) Mean λ, (W/(m·K))	Ävrö granite 12 samples (Laxemar + Simpevarp) Mean λ, (W/(m·K))
Calculated (SCA)	2.56[1]	2.34[2]	2.57[2]	2.82[2]
Measured (TPS)	2.85	2.62	2.68	3.06
Diff (SCA-TPS)/TPS	–10.1%	–10.8%	–4.1%	–7.67%

[1] Corrected for sericitisation and chloritisation. [2] No correction for sericitisation and chloritisation made.

Statistical tests were performed to compare the mean and variance for measured (TPS) and calculated (SCA) values of thermal conductivity. The paired t-test was applied to test for difference in the mean between TPS and SCA data. Tests were performed on samples from the same locations for rock type fine-grained dioritoid (501030) and Ävrö granite (501044). For Ävrö granite samples from Simpevarp and Laxemar significant differences in the mean were noted (5% significance level), see Figure 4-9. The results from Äspö were excluded since the SCA calculations were determined in a slightly different manner as compared to the data from Simpevarp and Laxemar. For fine-grained dioritoid the difference in mean between TPS and SCA data was significant but a significant difference in variance could not be detected /Sundberg et al. 2005b/.

Two-sample t-tests were performed on all TPS data (Laxemar, Simpevarp and Äspö) and SCA data (Laxemar and Simpevarp subareas) for different rock types, see Figure 4-10 to Figure 4-12. The tests indicate that there is a significant difference in the means derived by the different methods for fine-grained dioritoid (501030), quartz monzodiorite (501036), and Ävrö granite (501044). For all three rock types, the mean value of SCA calculations is lower than the mean value of TPS measurements implying that the SCA method is underestimating the thermal conductivity. The lower box plot in the figures illustrates the sample distribution, where the middle line of the box corresponds to the median, the start and end of the box the first and third quartile, the horizontal lines from the box are upper and lower whisker. Values beyond the whiskers are defined as outliers, and are marked by stars.

For 501030 the variance of TPS measurements is smaller than the variance of SCA calculations implying that the values are distributed within a smaller interval. The situation is different for rock type Ävrö granite (501044), and quartz monzodiorite (501036) where variances for TPS and SCA data are almost identical, i.e. no significant difference could be detected.

The systematic bias observed in the SCA calculations as compared to the TPS measurements can be explained by the following factors:

- Alteration. Alteration of plagioclase (sericitisation) and biotite (chloritisation) has been observed in samples throughout the Laxemar and Simpevarp subareas. The alteration products, sericite and chlorite, have higher thermal conductivities than their parent minerals. However, the point-counting procedure did not take the alteration products into account and therefore the effect of these minerals is not incorporated into the SCA calculations. This results in the thermal conductivities being underestimated. This is considered to be the main source of uncertainty.

- Anorthite content of plagioclase. As described above the thermal conductivity of plagioclase varies with its composition. Alteration of plagioclase, for example sericitisation and/or sausseritization, is commonly accompanied by the formation of albite, the sodium rich end-member of plagioclase (anorthite content = 0–10). As can be seen in Figure 4-6, plagioclase of this composition has considerably higher thermal conductivity than plagioclase with higher anorthite contents.

- Uncertainties exist regarding the reference values of thermal conductivity assigned to minerals, particularly those that display a range of compositions, for example amphibole. Even the different forms of alkali feldspar display different thermal conductivities /Horai 1971/. The effect of choosing a mean for the different forms of alkali feldspar (2.29 W/(m·K)) instead of a value based on orthoclase and microcline (2.40 W/(m·K)) is an underestimation of thermal conductivities in the order of 0.03 W/(m·K) for typical granitic rocks with 20% alkali feldspar.

- Errors associated with the point-counting method are another uncertainty which may produce biased SCA results.

It is possible that the calculation method (SCA) also contributes to the bias. However, based on present knowledge this is assumed not to be significant since its basis is a 3D approximation /Dagan 1979, Sundberg 1988/.

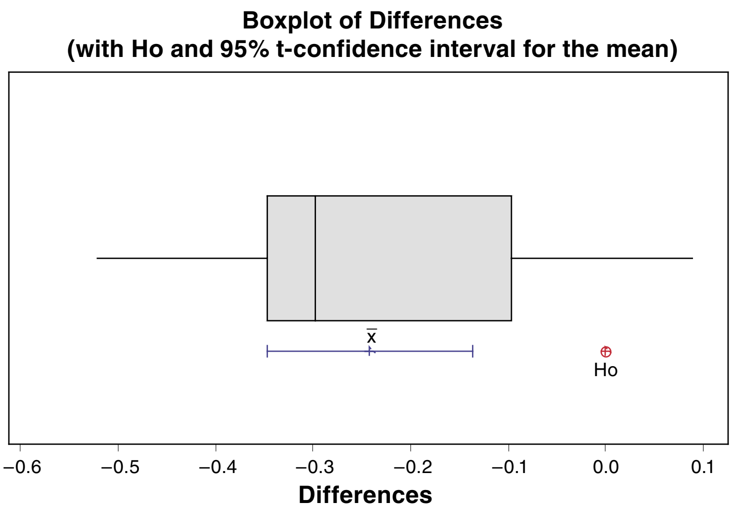

Figure 4-9. *Result of paired t- test for mean between TPS measurements and SCA calculations of thermal conductivity for rock type Ävrö granite (501044). n = 12. t-test of mean difference = 0 (vs not = 0): T-Value = –5.03 P-Value = 0.000.*

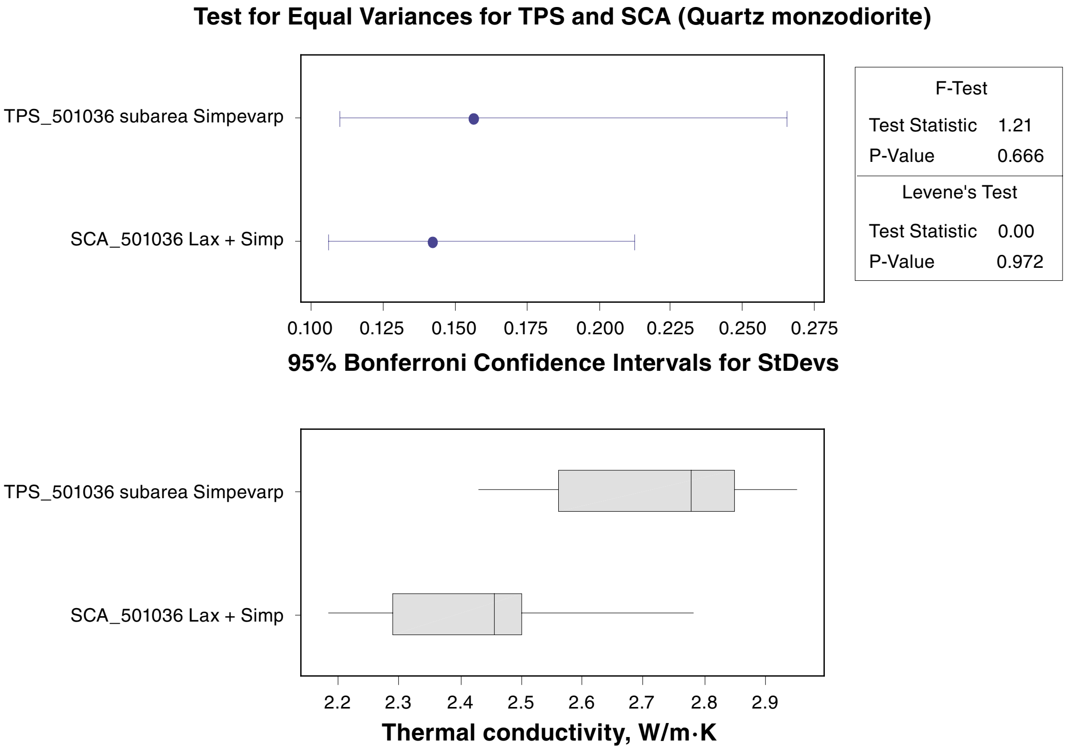

Figure 4-10. *Result of test for equal variances between all TPS measurements and SCA calculations of thermal conductivity for rock types Ävrö granite (501044) (F-test and Levene's test). Boxplots show the relationships between the mean of SCA calculations and TPS measurements for the rock type.*

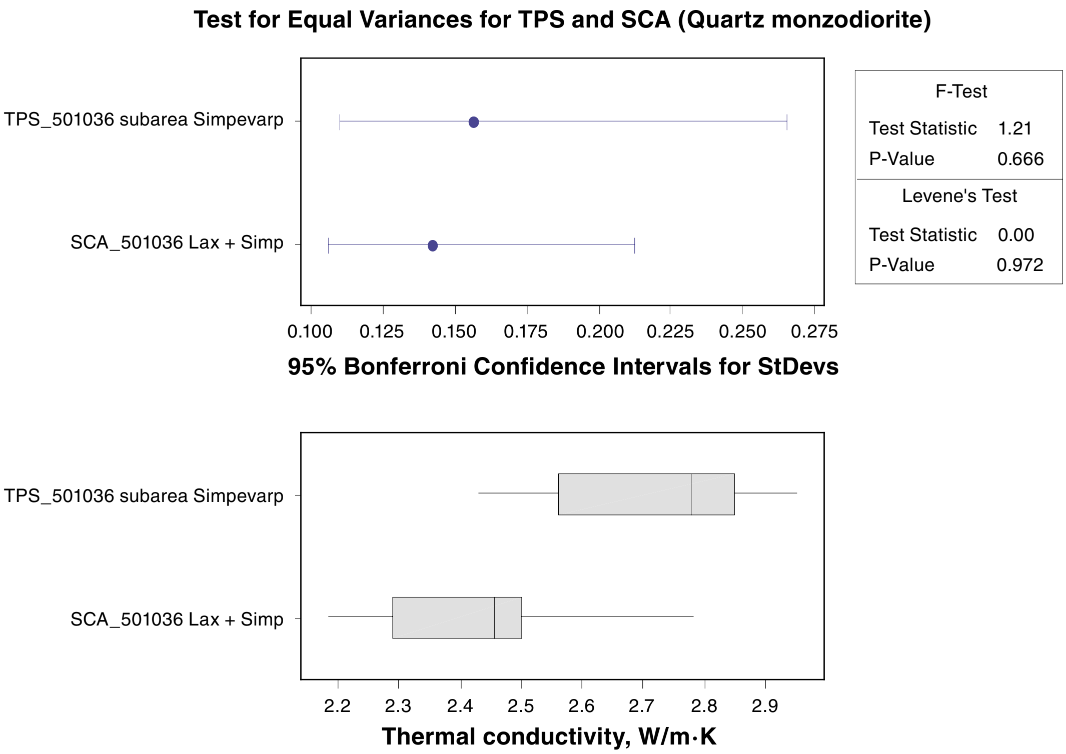

Figure 4-11. *Result of test for equal variances between all TPS measurements and SCA calculations of thermal conductivity for rock type quartz monzodiorite (501036) (F-test and Levene's test). Boxplots show the relationships between the mean of SCA calculations and TPS measurements for the rock type.*

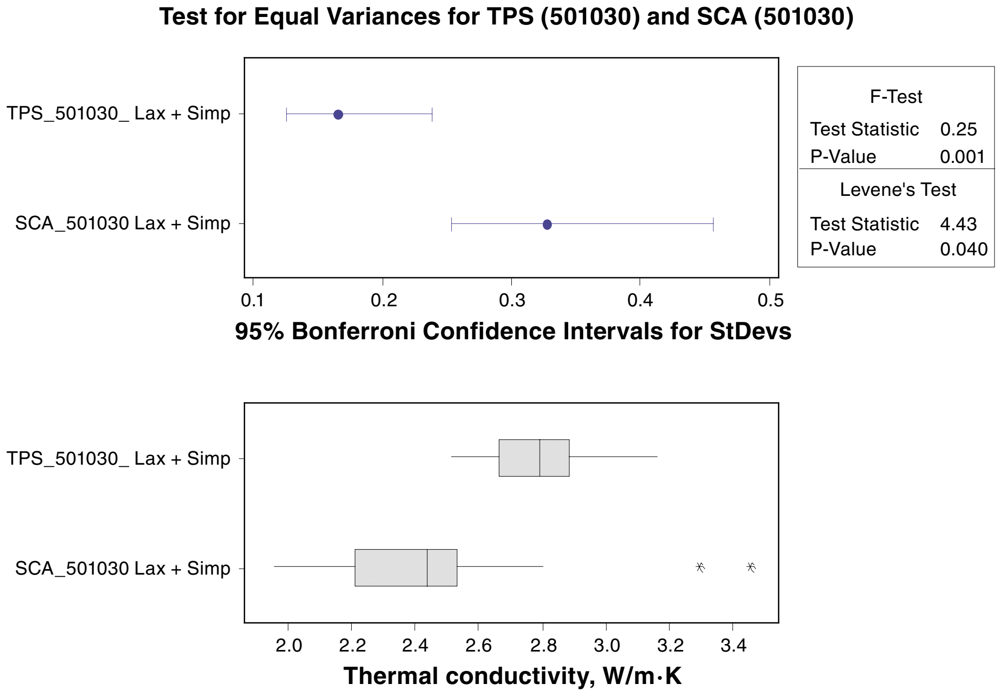

Figure 4-12. *Result of test for equal variances between all TPS measurements and SCA calculations of thermal conductivity for rock type fine-grained dioritoid (501030) (F-test and Levene's test). There is a significant difference in variance for fine-grained dioritoid (501030) as indicated by the low p-values. Boxplots show the relationships between the means of SCA calculations and TPS measurements for the rock type.*

4.5 Thermal conductivity from density

4.5.1 Method

In /Sundberg, 2003b/ an equation of the relationship between density and measured (TPS) thermal conductivity for 20 samples of Ävrö granite (501044) was found and presented. An improved relationship using additional measurements (37 in total) was presented in /Sundberg et al. 2005b/, but also below in Equation 4-1 and Figure 4-13.

$y = -0.0071668x+22.326$ $\qquad R^2 = 0.74$ $\qquad$ *Equation 4-1*

A total of 34 new measurements were produced for the Laxemar model version 1.2. These samples are from boreholes KLX02, KLX04 and KAV04A. A new relationship based on previous data together with the results from the recent measurements has been developed.

The relationship between density and thermal conductivity, for Ävrö granite (501044), based on all available data is:

$y = -0.0076021x+23.507$ $\qquad R^2 = 0.81$ $\qquad$ *Equation 4-2*

Figure 4-14 illustrates a plot of thermal conductivity against density for all rock types for which data is available. No unequivocal relationship between thermal conductivity and density is apparent within the other investigated rock types. There are as yet no data for mafic rock types. Note that the data for quartz monzodiorite is derived from only three different localities. Each locality produces its own distinct cluster of data points.

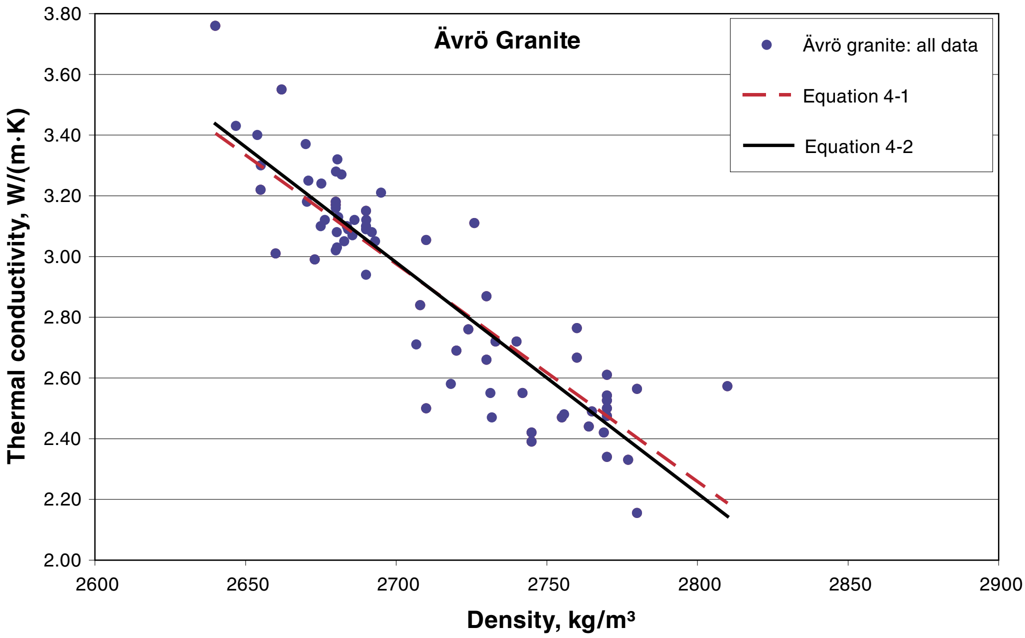

Figure 4-13. *Relationships between density and thermal conductivity (TPS measurements). Based on linear regressions, Equation 4-1 is the relationship from /Sundberg 2005b (S1.2)/ and Equation 4-2 is the relationship used in this study. The validity of both relationships is limited to rock type Ävrö granite (501044) and data from the other rock types are not used in the regression.*

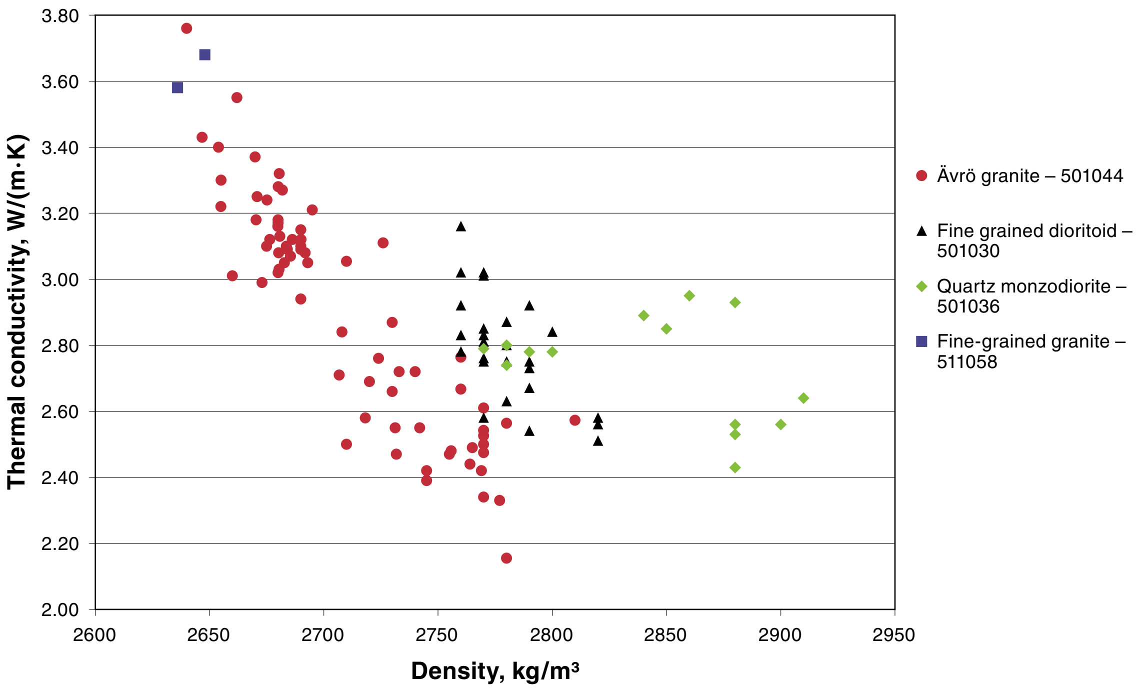

Figure 4-14. *Relationships between density and thermal conductivity for four rock types.*

The model for Ävrö granite (relationship between density and thermal conductivity) has been evaluated statistically by calculating both the confidence interval and prediction interval. The confidence interval, marked in Figure 4-15 with a red dashed line, indicates the uncertainty of the model. The interval can be interpreted as the area the model will fall within with 95% probability. The prediction interval marked in Figure 4-15 with a green dashed line shows the uncertainty in predicting thermal conductivity from a density measurement. The interval can be interpreted as the area a prediction of the thermal conductivity will fall with 95% probability. As Figure 4-15 indicates, the prediction interval is much wider than the confidence interval, implying the model fitted to data is less uncertain than a prediction of thermal conductivity from density measurement.

4.5.2 Results

Based on the relationship between density and thermal conductivity derived for Ävrö granite as explained in the previous Section 4.5.1, density values given by the density loggings of boreholes KAV04, KLX01, KLX02, KLX03 and KLX04, were used to deterministically assign a thermal conductivity value to each logged decimetre section of Ävrö granite. The density loggings for these boreholes are illustrated in Figure 4-16 to Figure 4-20. The rock types (occurrences > 1 m) are displayed as lithological columns.

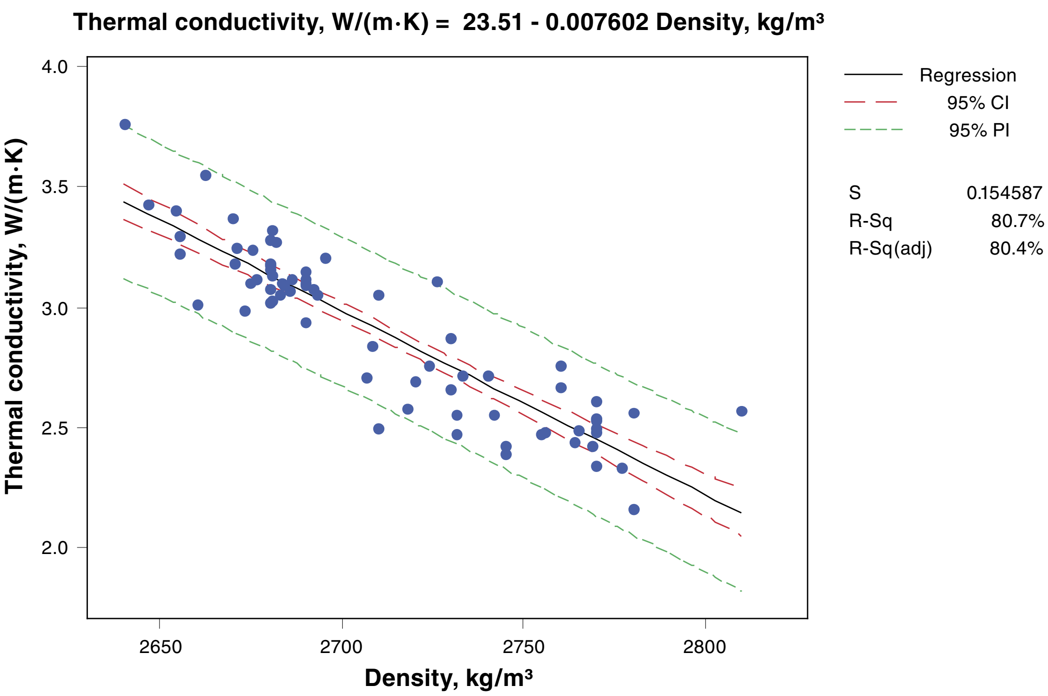

Figure 4-15. Statistical analysis of the relationship between density and thermal conductivity for rock type Ävrö granite (501044). The red lines indicate the confidence interval for the model and the green lines the prediction interval.

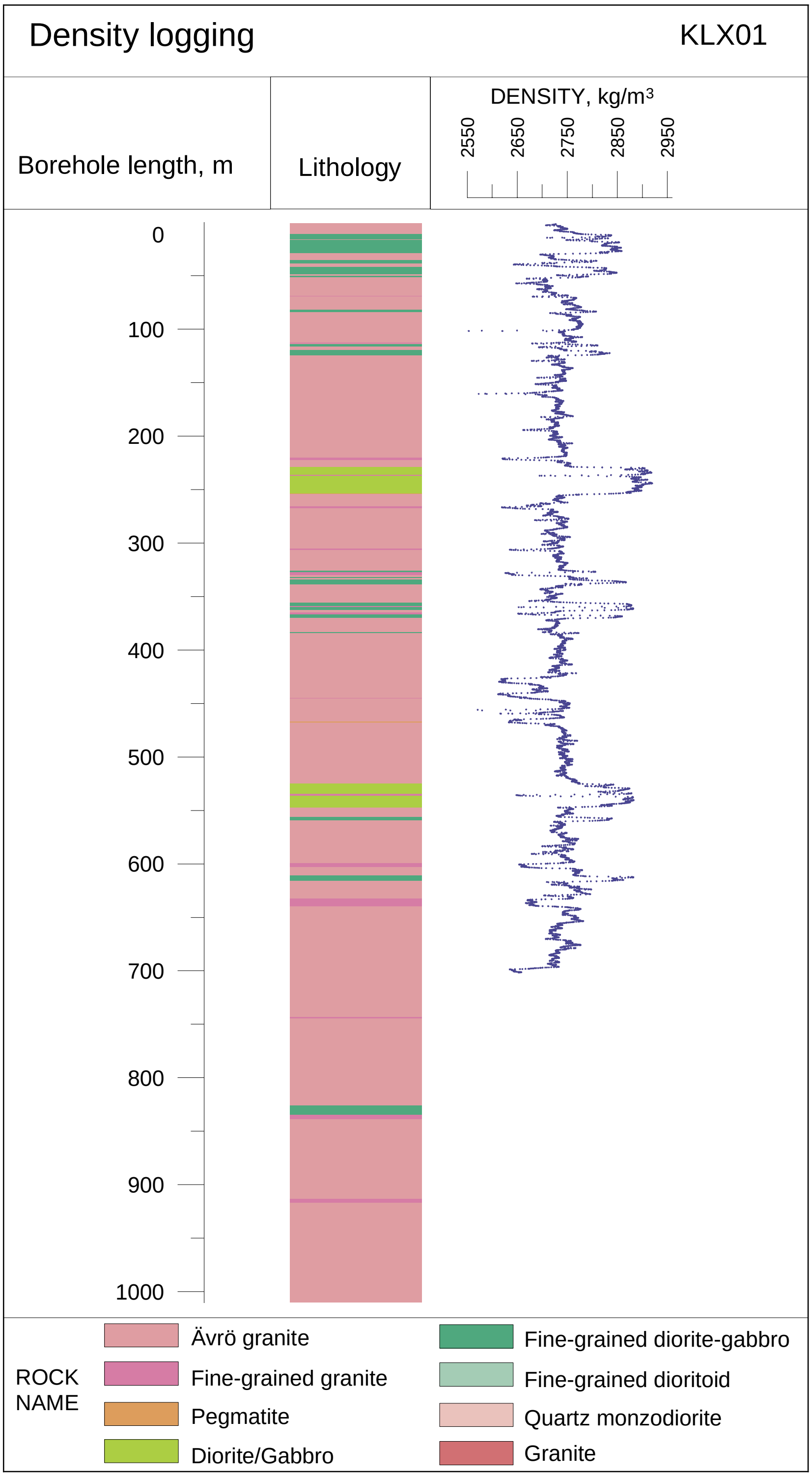

Figure 4-16. *Lithology and density log for borehole KLX01.*

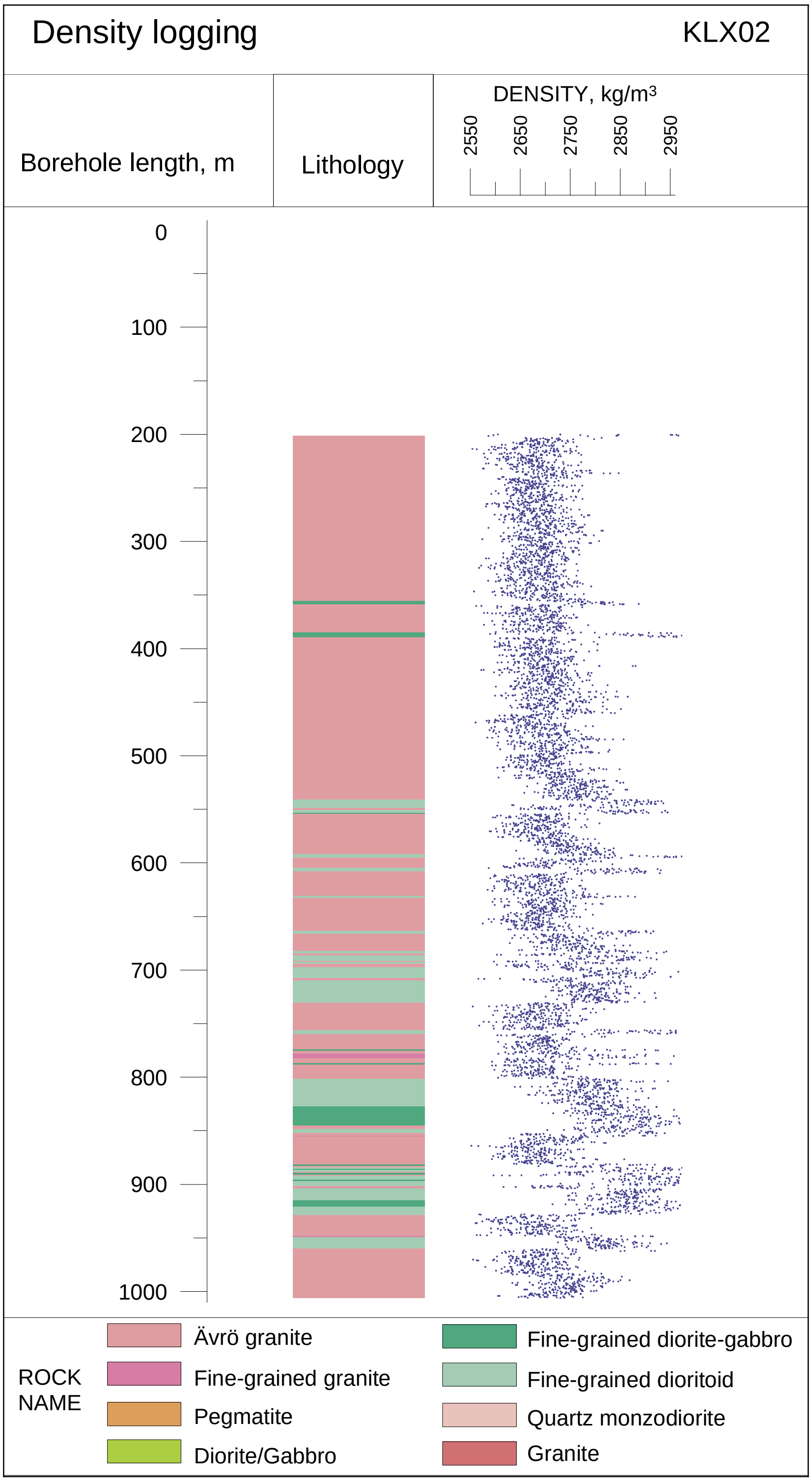

Figure 4-17. *Lithology and density log for borehole KLX02.*

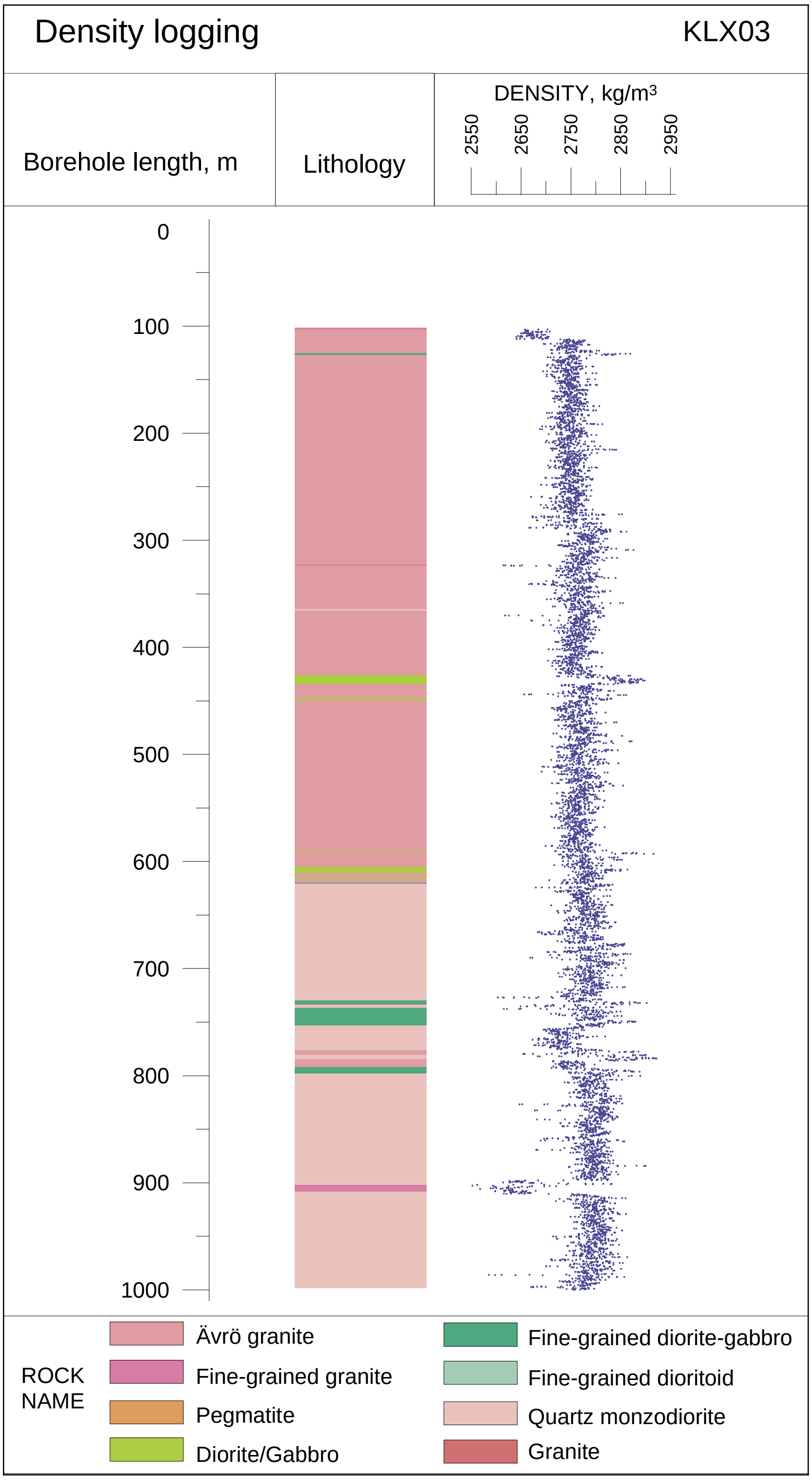

Figure 4-18. *Lithology and density log for borehole KLX03.*

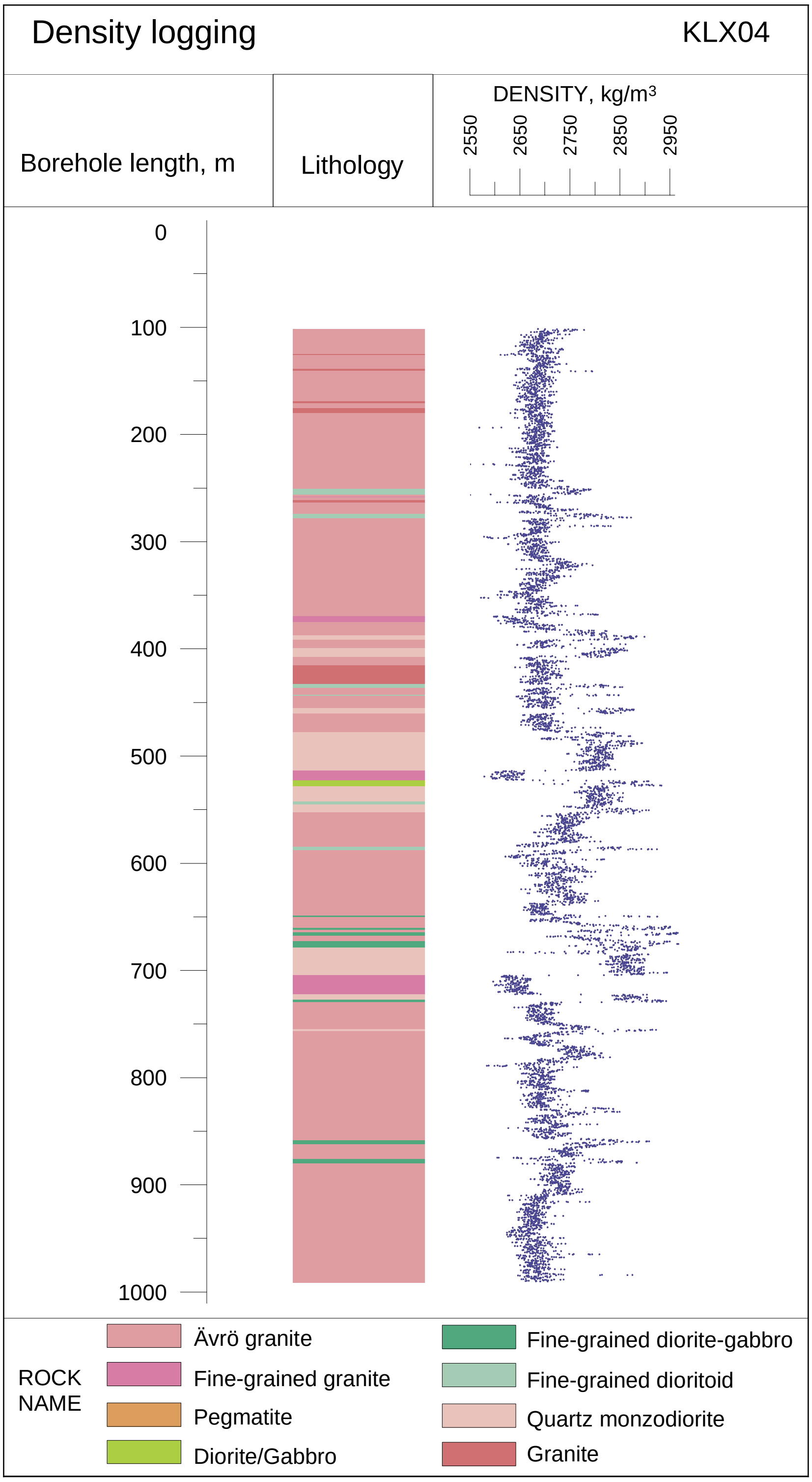

***Figure 4-19.** Lithology and density log for borehole KLX04.*

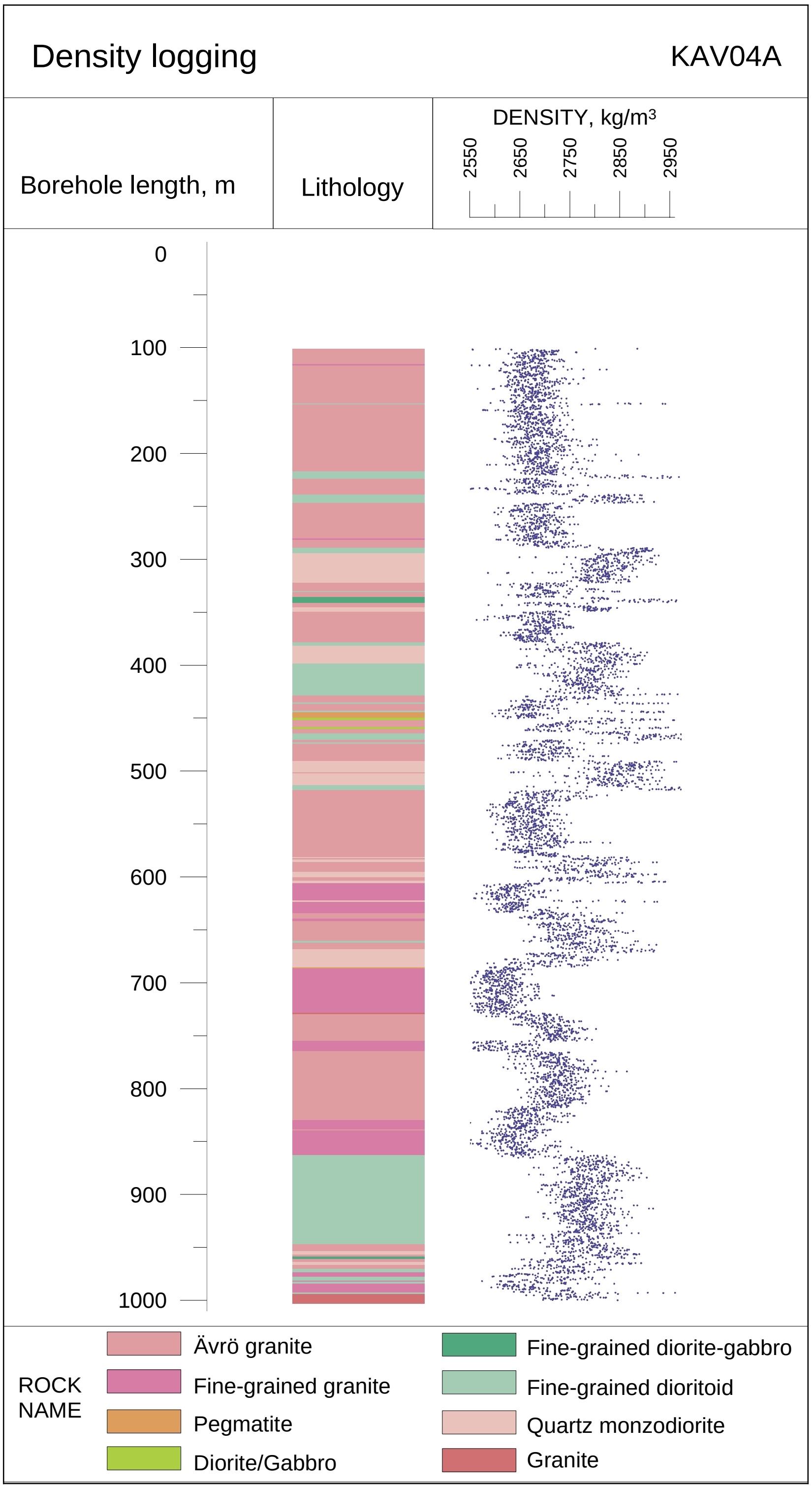

***Figure 4-20.** Lithology and density log for borehole KAV04A.*

Density logging data for all boreholes were re-sampled, calibrated and filtered /Mattsson 2004ab/ and /Mattsson et al. 2005/. The re-sampling is done to make sure that all logging methods have values for the same common depth co-ordinate with exactly 0.1 m point distance. Calibration deviates somewhat from the procedure used for the data in Simpevarp 1.2. Data from Ävrö granite from 6 boreholes (KAV04, KLX01, KLX02, KLX03, KLX04 and KSH01A) was used to establish a correlation equation between logged data and measured core samples. The calibration, carried out by GeoVista /Mattsson 2005/, has been done by fitting a regression line to a crossplot of density logging data versus density data from core samples. Finally the logged data was filtered using a 3-point average filter to reduce the effect of high-frequency measurement noise. It should be noted that the data for KLX01, which was logged by a different company in 1993, displays much less background noise than the other boreholes.

When the relationship between density and thermal conductivity is applied to density loggings of KAV04, KLX01, KLX02, KLX03 and KLX04 the distribution of thermal conductivity within the boreholes can be illustrated, see Figure 4-21 for example. For the purposes of modelling thermal conductivity from density loggings, it is assumed that the established relationship is valid within the density interval 2,600–2,850 kg/m^3, which corresponds to the thermal conductivity interval 1.84–3.74 W/(m·K), i.e. slightly outside the interval of measured data. The extreme, both high and low, values of thermal conductivity produced are purely an effect of the considerable random noise in the density loggings. It is still considered justified to extrapolate the density relationship within this interval since, firstly these extreme values tend to disappear as a consequence of upscaling, and secondly using a more restricted density range would produce a systematic bias in the results. Table 4-14 summarises the results of the measurements for each borehole.

The frequency histograms in Figure 4-22 display the distribution of thermal conductivity values calculated from density loggings for each borehole. When data from all boreholes are combined, it appears (Figure 4-23) that the distribution of thermal conductivity calculations for Ävrö granite contains two modes, one at 2.7 W/(m·K) and one at 3.05 W/(m·K). However, others modes may be present. This seemingly bimodal distribution is also evident in both the TPS and SCA data sets for Ävrö granite. A comparison of the distributions from the individual boreholes reveals two broadly different groups; one group represented by boreholes KLX02, KLX04 and KAV04A, the other by boreholes KLX01 and KLX03, see Figure 4-24 and Figure 4-25. The latter group has lower mean thermal conductivities and lower standard deviations that the former.

Table 4-14. Summary of density logging of Ävrö granite per borehole.

Borehole	% Ävrö granite in borehole	No of measurements within density interval 2,600–2,850 kg/m^3	% measurements excluded (outside model interval)	Logged borehole interval	Thermal conductivity, W/(m·K) – Mean (Std dev)
KAV04A	50.24	4,444	1.7%	101.0–1,002.2 m	3.01 (0.34)
KLX01	80.03	5,586	0.4%	1.0–701.6 m	2.77 (0.20)
KLX02	70.88	5,499	3.4%	201.5–1,004.9 m	3.02 (0.36)
KLX03	54.18	4,829	0.8%	101.8–999.9 m	2.57 (0.21)
KLX04	72.23	6,369	0.8%	101.6–990.2 m	3.02 (0.27)
All boreholes		26,727			2.88 (0.33)

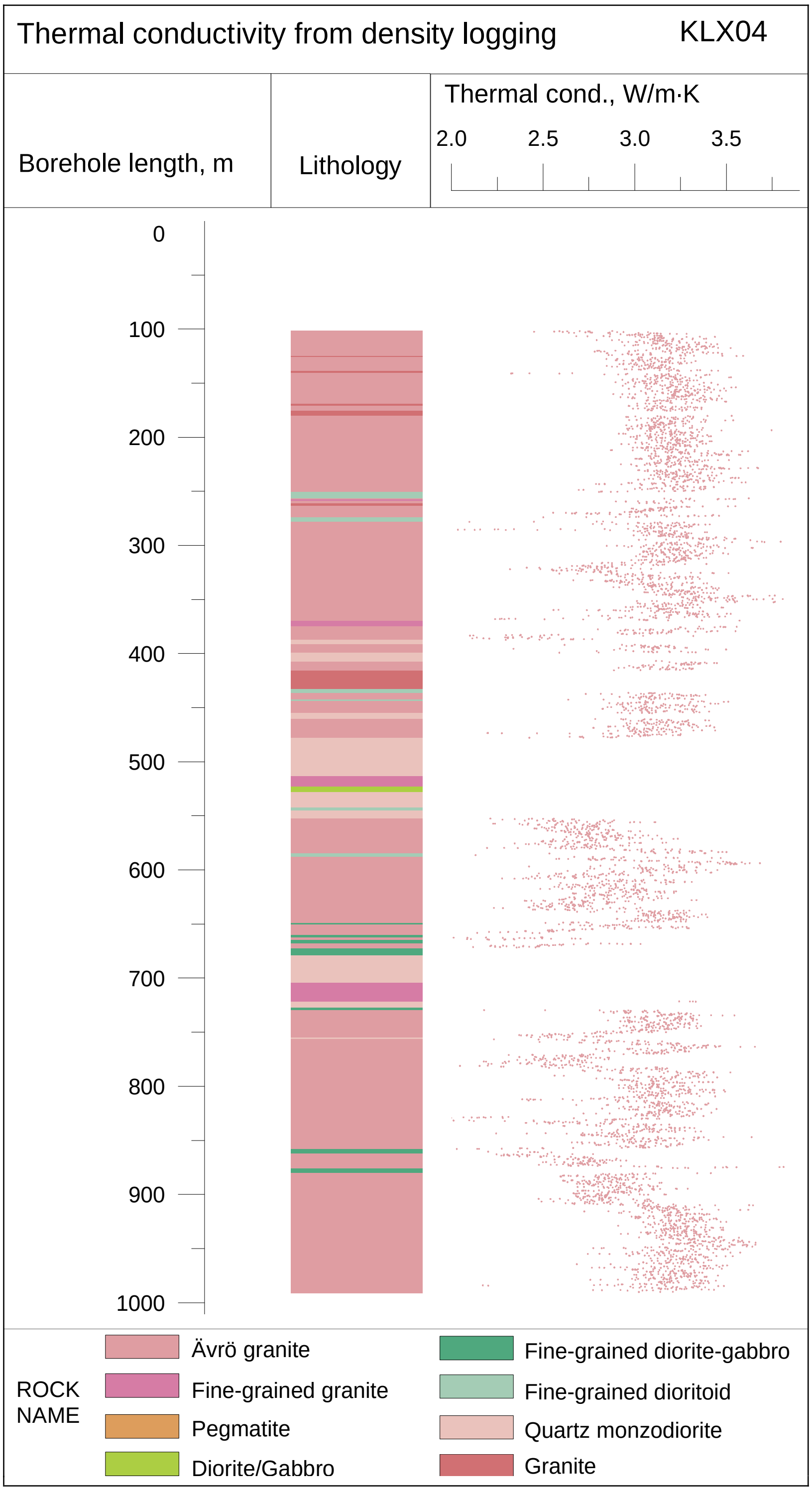

Figure 4-21. *Thermal conductivity of Ävrö granite (501044) in KLX04A estimated from density logging alongside a generalised geological borehole log.*

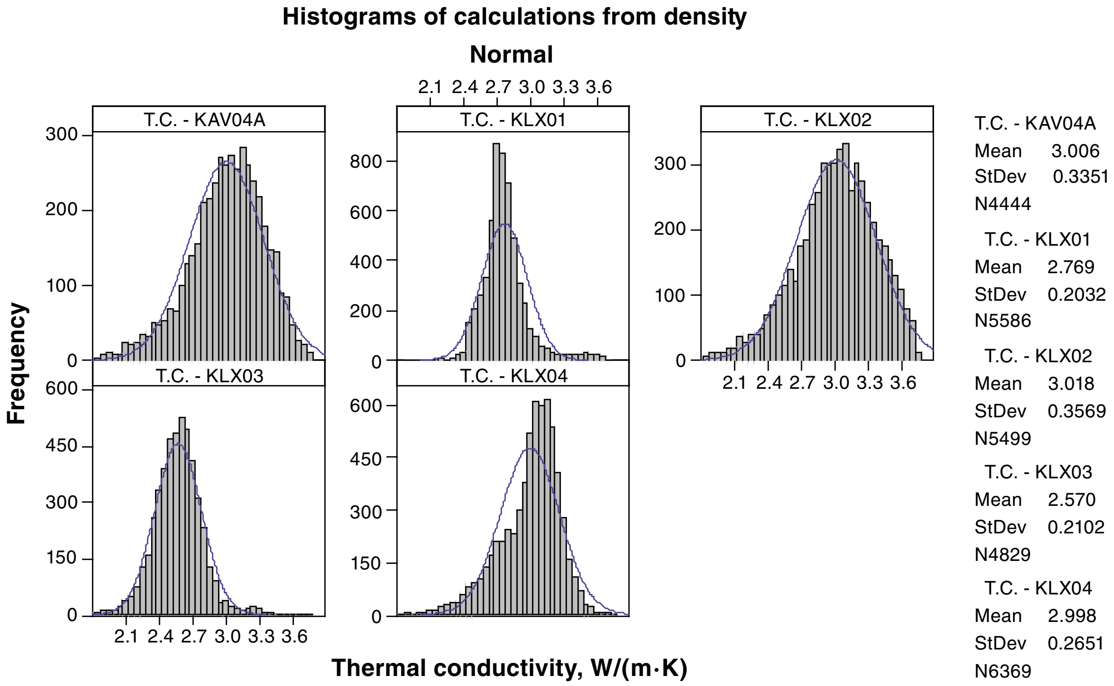

Figure 4-22. *Histograms of thermal conductivities for Ävrö granite calculated from density loggings for boreholes KAV04A, KLX01, KLX02, KLX03, and KLX04. Normal distribution curves fitted.*

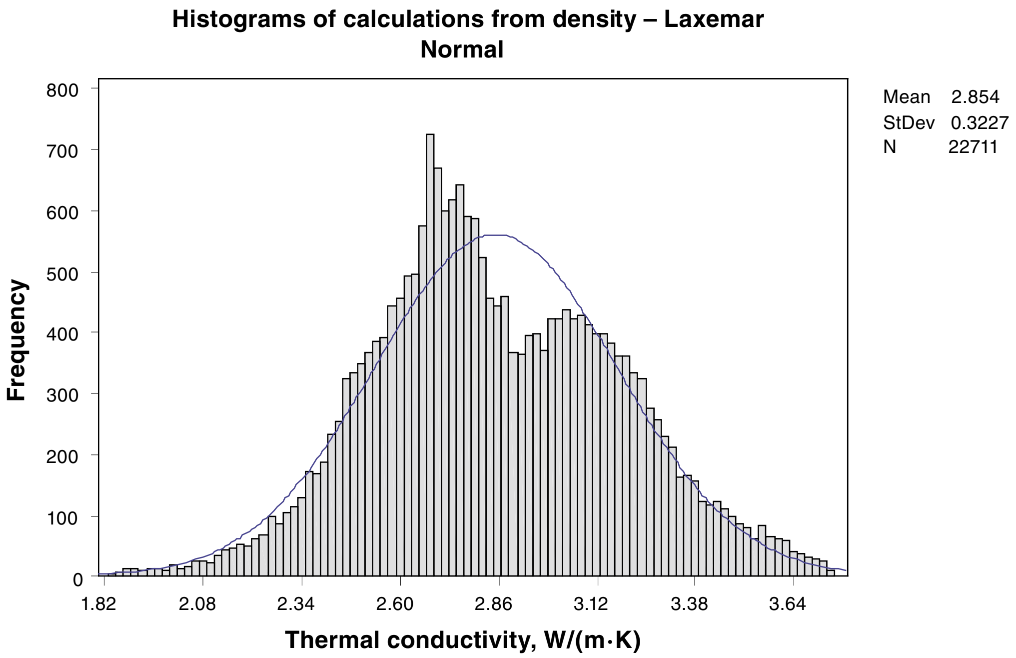

Figure 4-23. *Histogram of thermal conductivities for Ävrö granite calculated from density loggings for boreholes KAV04A, KLX01, KLX02, KLX03, and KLX04. Normal distribution curves fitted.*

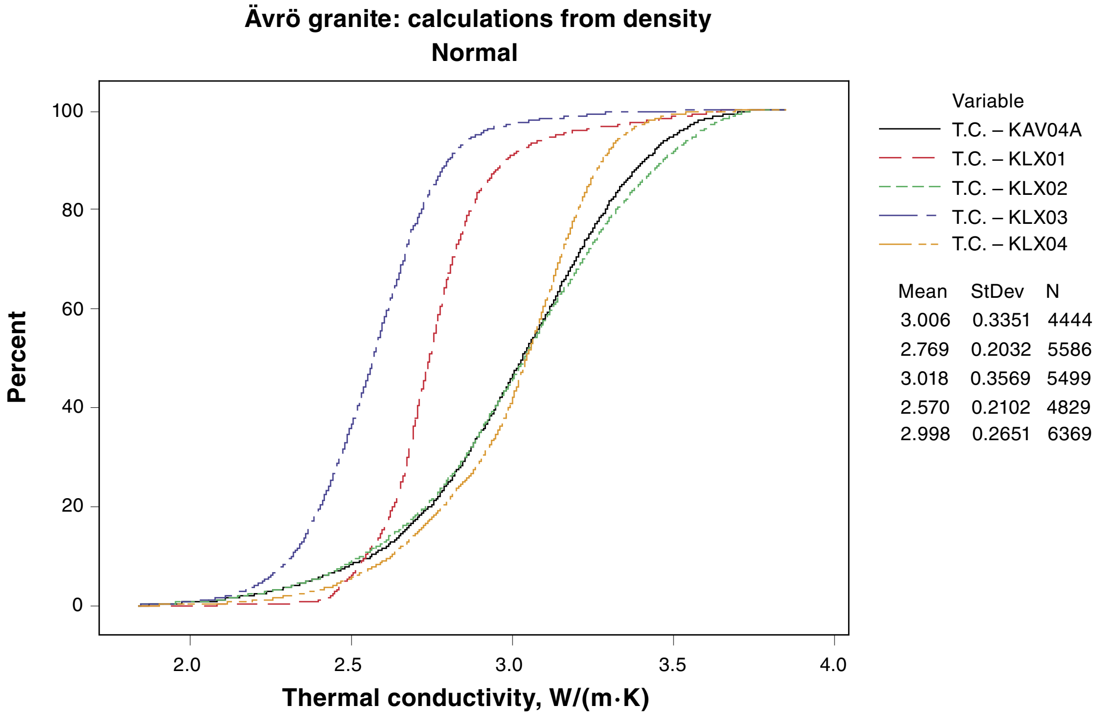

Figure 4-24. *Cumulative frequency plot of thermal conductivities for Ävrö granite calculated from density loggings for boreholes KAV04A, KLX01, KLX02, KLX03, and KLX04.*

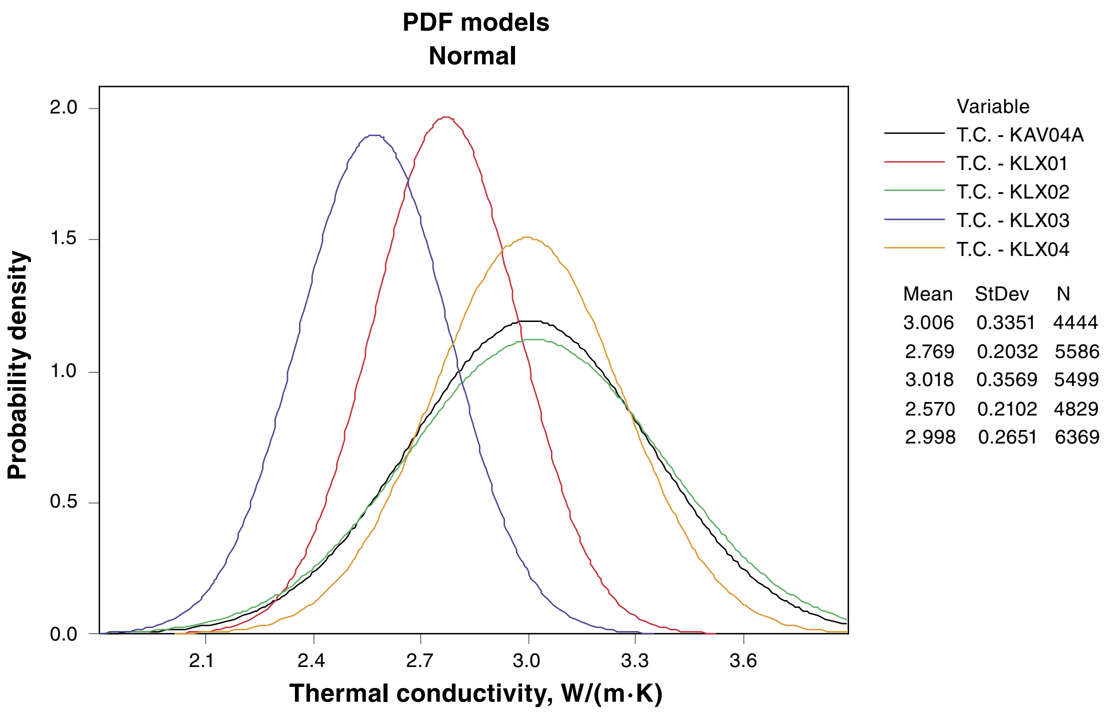

Figure 4-25. *PDF:s of thermal conductivities for Ävrö granite calculated from density loggings for boreholes KAV04A, KLX01, KLX02, KLX03, and KLX04.*

It should be noted that the data distribution diagrams below refer to data at the 0.1 m scale. At this scale the lowest and highest values are likely to be an effect of the noise in the density loggings, and probably do not occur in reality. These are evened out, however, as a result of upscaling, see chapter 5.

Thermal conductivities calculated from density loggings for boreholes KSH01A, KAV01 and KLX02 were presented in Simpevarp model version 1.2. The mean and standard deviation of the data population were 2.96 W/(m·K) and 0.36 W/(m·K) respectively. When the entire data set is considered, no significant difference between the Laxemar and Simpevarp subareas is indicated.

4.5.3 Comparison between measurements and calculations

In order to evaluate how well the model in Equation 4-2 (cf Figure 4-13) reflects the actual thermal conductivity in the borehole, measured samples (TPS) were compared with values estimated from density logging. Direct density measurements on samples and density loggings from the corresponding borehole interval have also been compared.

For measurement by the TPS method, 35 samples of Ävrö granite from boreholes KAV04A, KLX02 and KLX04 were taken in 12 groups, each group comprising a number of samples from a short (< 1 m) length of borehole. The density of these samples was also determined. For the same sections of the borehole the thermal conductivity and density was calculated from density logging and by Equation 4-2. The results of the comparisons are presented in Table 4-15 and Table 4-16. In relation to laboratory measurements, the density loggings underestimate the thermal conductivity by on average 1.78%, which is equivalent to

Table 4-15. Comparison of thermal conductivity (W/(m·K)) measured with the TPS method in Ävrö granite vs calculated thermal conductivity from density logging of the same borehole intervals.

Borehole	Borehole interval: (Secup–Seclow), m	TPS, mean	Diff (max-min)	No of samples	Thermal cond. from density logging, mean	Diff (max-min)	No of measurements	Diff (Density logging-TPS)/TPS
KAV04A	521.45–521.80	3.10	0.43	5	3.09	0.35	5	–0.60%
KLX02	314.33–314.63	3.15	0.21	5	3.14	0.80	5	–0.33%
KLX02	492.30–492.42	3.07	0.03	2	2.56	0.37	2	–16.36%
KLX02	501.95–502.13	3.22	0.20	3	3.43	0.06	3	6.40%
KLX02	738.22–738.34	3.18	0.15	2	3.09	0.27	3	–2.66%
KLX02	740.02–740.20	3.06	0.07	3	2.84	0.37	3	–7.06%
KLX04	308.14–308.26	3.15	0.06	2	3.03	0.13	3	–3.75%
KLX04	312.34–312.52	3.38	0.13	3	3.22	0.13	4	–4.73%
KLX04	562.08–562.20	2.65	0.13	2	2.69	0.16	3	1.76%
KLX04	567.20–567.37	2.50	0.08	3	2.70	0.14	3	7.81%
KLX04	739.48–739.66	3.17	0.19	3	3.14	0.24	4	–0.84%
KLX04	746.39–746.51	3.19	0.16	2	3.15	0.19	4	–1.02%
							Mean diff =	–1.78%

Table 4-16. Comparison of density (kg/m³) measurements on core samples in Ävrö granite and measurements by density logging of the same borehole intervals.

Borehole	Borehole interval: (Secup–Seclow), m	Density measurements, mean	Diff (max-min)	No of samples	Density from density logging, mean	Diff (max-min)	No of measurements	Diff (Density logging-meas.)/meas.
KAV04A	521.45–521.80	2,684	20	5	2,686	46	5	0.09%
KLX02	314.33–314.63	2,686	15	5	2,678	105	5	–0.28%
KLX02	492.30–492.42	2,692	1	2	2,754	48	2	2.32%
KLX02	501.95–502.13	2,681	17	3	2,642	8	3	–1.48%
KLX02	738.22–738.34	2,672	4	2	2,685	36	3	0.48%
KLX02	740.02–740.20	2,682	3	3	2,718	49	3	1.33%
KLX04	308.14–308.26	2,673	6	2	2,693	17	3	0.75%
KLX04	312.34–312.52	2,651	8	3	2,669	17	4	0.64%
KLX04	562.08–562.20	2,712	11	2	2,738	21	3	0.95%
KLX04	567.20–567.37	2,739	25	3	2,737	19	3	–0.07%
KLX04	739.48–739.66	2,680	2	3	2,678	31	4	–0.08%
KLX04	746.39–746.51	2,677	6	2	2,677	25	4	–0.02%
							Mean diff = 0.39%	

0.06 W/(m·K). Samples with high conductivity values are strongly overrepresented in the comparison, so that the observed bias may not apply to low conductivity varieties of Ävrö granite. On the contrary, the two samples of low thermal conductivity Ävrö granite (KLX04, 562 and 567 m) indicate that the values estimated from density logging may be overestimating the true thermal conductivity in the low conductivity range for this rock type. More laboratory measurements are required for verification of the method for low conductivity Ävrö granite.

The average difference in mean density calculated by the two separate methods (Table 4-16) is 0.39%, implying that the logging data is overestimating density. In terms of thermal conductivity this is equivalent to values that are too low by about 0.08 W/(m·K).

4.6 Statistical rock type models of thermal conductivity

4.6.1 Method

There are different data sets of thermal conductivity for the dominant rock types. The most reliable data comes from TPS measurements but these samples may not be representative of the rock type due to the limited number of samples and the sample selection procedure. Samples on which SCA calculations are based have a larger spatial distribution in the rock mass.

Rock type models (Probability Density Functions, PDF:s) of thermal conductivity have, with the exception of Ävrö granite, been produced by combining the available data from TPS measurements and SCA calculations from mineral composition. For some rock types only SCA calculations are available. The SCA calculations of rock types fine-grained dioritoid (501030) and quartz monzodiorite (501036) have been corrected in order to reduce the effect of a potential bias in the SCA calculations according to Table 4-13. For both rock types, a correction by a factor of 1.10 is applied. For quartz monzodiorite (501036) this is a departure from the procedure followed in Simpevarp model version 1.2, where without sufficient data no correction of the SCA data was deemed justifiable. SCA data for Ävrö granite (501044) were used in the construction of a rock type model in Simpevarp 1.2, but because of the availability of additional TPS measurements it has been decided to exclude the SCA data from the model in this report. In Simpevarp 1.2 the SCA data for Ävrö granite was adjusted by a factor of 1.04. Assessment of the newly available SCA data from Simpevarp and Laxemar indicates a correction by a factor of 1.08, which in previous Section 4.4.3 has been shown as the difference between the two methods.

The rock type models are used to model thermal properties for lithological domains, see Section 5. Density loggings have not been used for the rock type models, but are applied in the domain modelling in order to include spatial variability. All rock types are assumed to be characterised by normal (gaussian) PDF:s. For Ävrö granite this assumption is unlikely to hold true. The available data for this rock type displays a bimodal distribution. However, this is only of minor importance in the modelling work which follows, since thermal conductivities for this this rock type are calculated from the density loggings rock type are generally calculated less than 3% of the Ävrö granite in the boreholes are modelled according to this distribution model. Thermal conductivities for the greater part of. Probability plots, assuming normal distribution of thermal conductivities, are illustrated in Figure 4-26 and lognormal distributions in Appendix A.

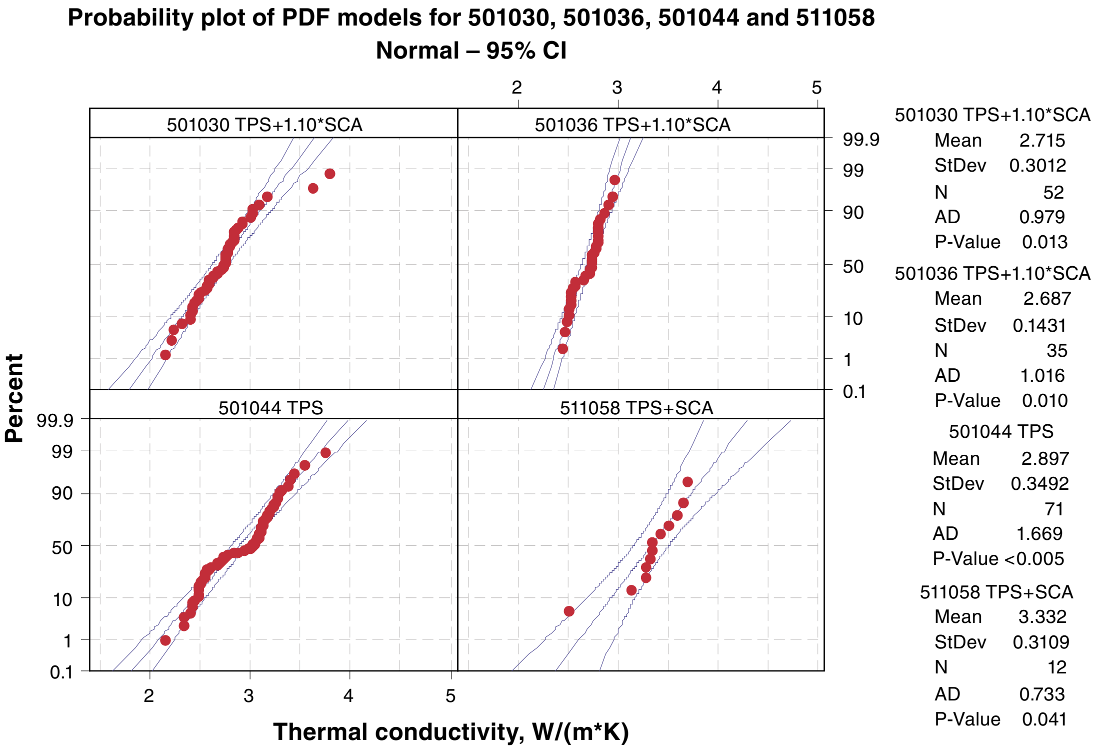

Figure 4-26. *Probability plots (normal distributions) of thermal conductivity according to rock types. For rock types fine-grained dioritoid (501030) and quartz monzodiorite (501036), the SCA calculations have been corrected by a factor of 1.10.*

4.6.2 Ävrö granite (501044)

For rock type Ävrö granite there are three sources of thermal conductivity data, SCA calculations from mineral compositions (modal analyses), TPS measurements and density loggings using the relationship presented in Section 4.5. Data from the three methods are summarised in Table 4-17. Figure 4-27 displays the characteristic bimodal distribution of TPS and SCA data, which in turn reflects the spatial variations in mineral composition present within this rock type /SKB 2006/. Although the number of samples on which the TPS data are based is rather large (n = 71), there may still be a problem of representativity. This is because samples have been taken from relatively few locations. Distribution models (PDF:s) based on data from the different methods are presented in Figure 4-28 and Table 4-17. A rock type model of the thermal conductivity for Ävrö granite (501044), used in the lithological domain modelling, is based solely on TPS measurements. A normal distribution is applied to TPS measurements, although cumulative histograms (Figure 4-30) indicate that the distribution is bimodal. The models based on SCA calculations and density logging are included for comparison. In Simpevarp 1.2 a combination of both TPS measurements and SCA calculations were employed in construction of the rock type model.

In Figure 4-29 and Figure 4-30 empirical cumulative distribution functions with fitted models (normal distributions) of rock type Ävrö granite (501044) are presented. The means of the data from the density loggings and data from TPS measurements show a rather good correspondence, in contrast to that found in Simpevarp 1.2 in which density loggings data had a higher mean than TPS data. Thermal conductivity from density loggings has been calculated for data from boreholes KAV04, KLX01, KLX02, KLX03 and KLX04. Data for boreholes KSH01A and KAV01 were presented in Simpevarp 1.2. Calculations from density data summarised in the table below derives solely from the Laxemar subarea.

SCA calculations are presented here for comparison but are not used in the rock type model. In this data set 13 samples have been excluded since both the SCA and TPS methods give a thermal conductivity of the same sample. (Samples from Äspö have also been excluded for reasons already mentioned.)

Table 4-17. Three different distributions of thermal conductivity (W/(m·K)) for rock type Ävrö granite (501044), based on different methods together with the rock type model.

	TPS measurements	Calculations from mineral composition	Calculations from density loggings	Rock type model
Mean	2.90	2.66	2.85	2.90
Std dev	0.35	0.30	0.32[1]	0.35
Number of samples	71	73	22,711	
Comment	Including samples from Äspö HRL.	Comparable samples indicates correction 8%.	Based on data from boreholes KLX01, KLX02, KLX03 and KLX04.	TPS measurements only

[1)] The variance is a consequence of the restricted validity interval for the density vs thermal conductivity relationship.

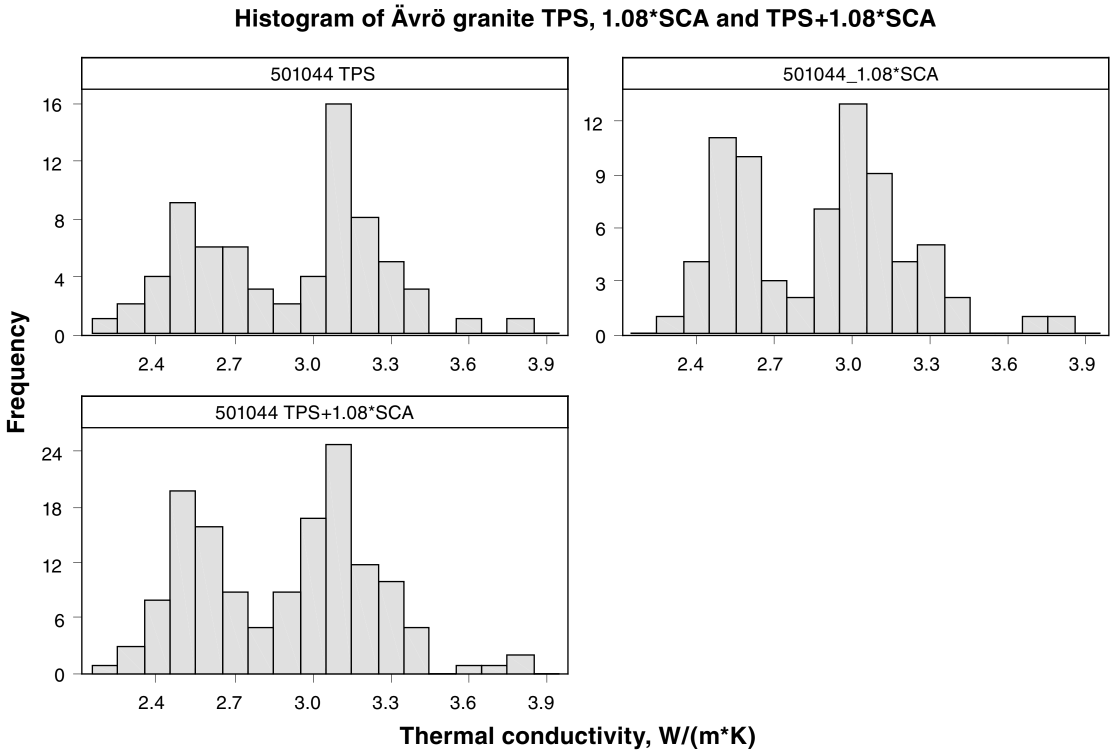

Figure 4-27. *Histograms for measured values (TPS), calculated values (SCA) and TPS plus SCA for rock type Ävrö granite (501044) showing a distinct bimodal distribution*

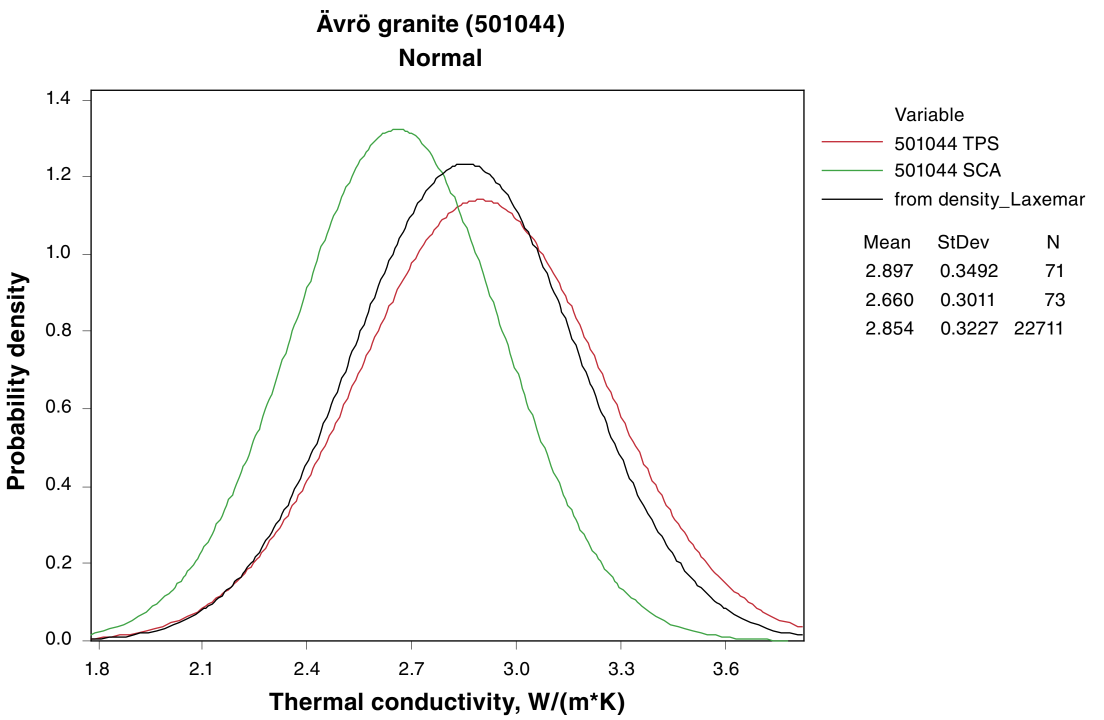

Figure 4-28. *PDF:s for measured values (TPS), calculated values (SCA),and density logging for rock type Ävrö granite (501044). The rock type model is based on TPS data. Data from the density loggings and TPS data have similar mean values.*

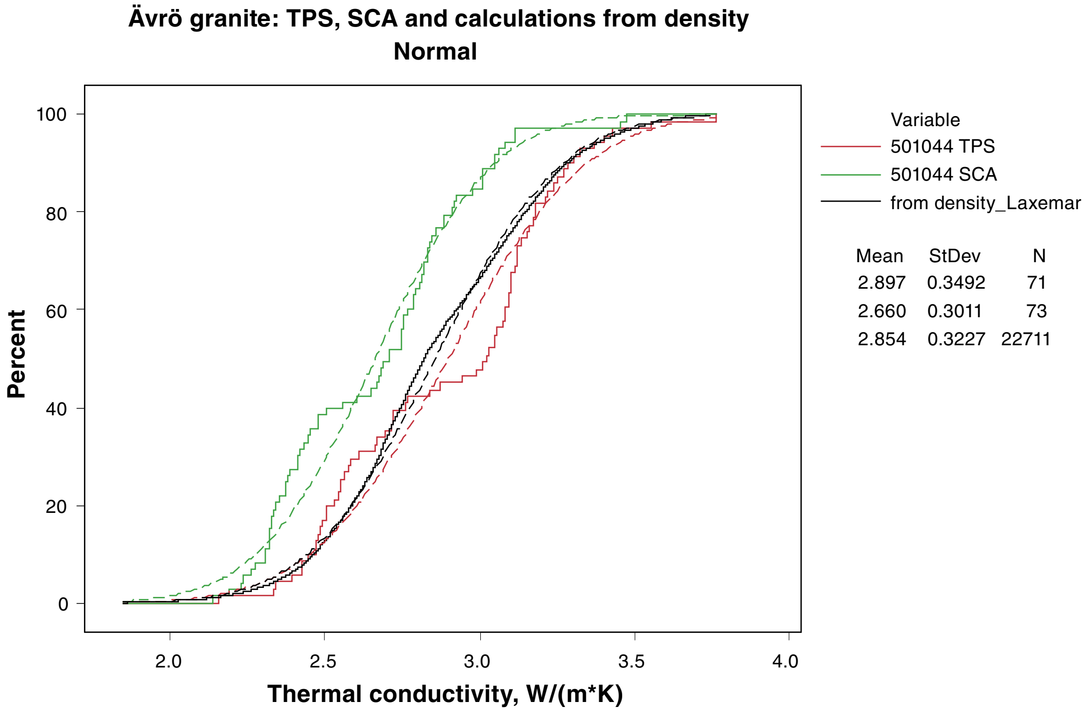

Figure 4-29. *Cumulative histogram of Ävrö granite (501044) with data from three sources, calculated from density loggings, TPS measurements and SCA calculations from mineral composition.*

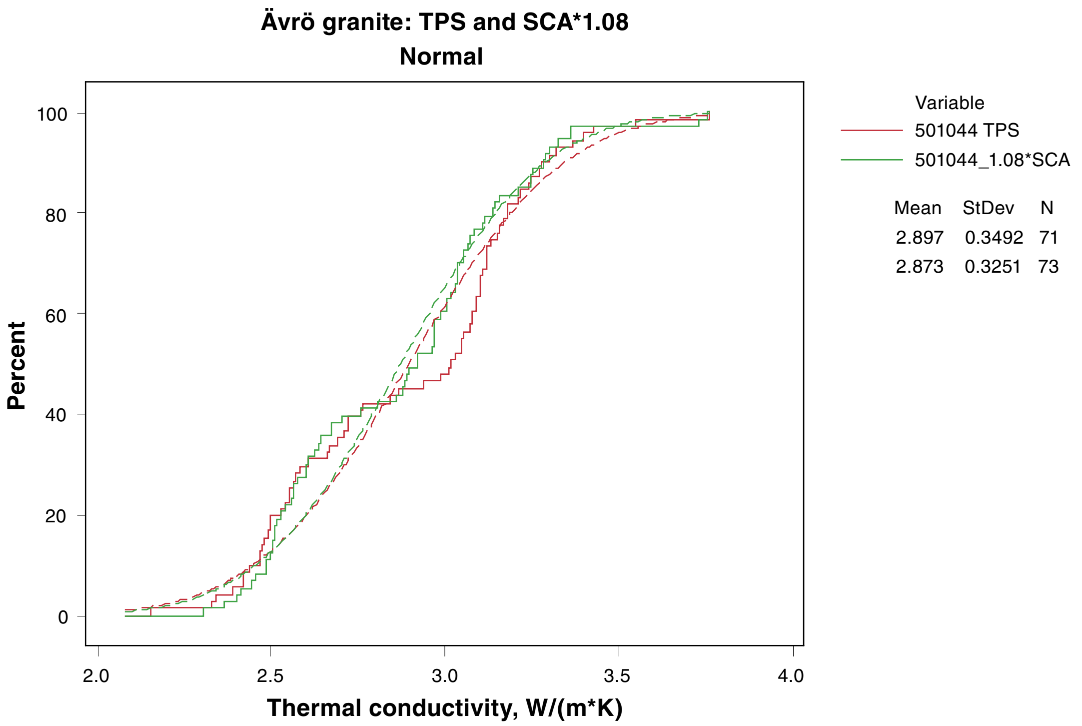

Figure 4-30. *Cumulative histogram of Ävrö granite (501044) with thermal conductivity calculated from corrected SCA and the rock type model based on TPS data.*

4.6.3 Quartz monzodiorite (501036)

For rock type quartz monzodiorite (501036) there are two sources of thermal conductivity data, SCA calculations based on mineral composition and TPS measurements. The data derives from both Laxemar and Simpevarp subareas; results from Äspö HRL are excluded. Data from the two methods are summarised in Table 4-18. Distribution models (PDF:s) based on data from the different methods, in addition to the rock type model, are presented in Figure 4-31 and Figure 4-32. As can be seen from the distribution functions, the two methods results in different mean values and variances. Figure 4-32 presents empirical cumulative distribution functions with fitted models (normal distributions) of rock type quartz monzodiorite (501036).

SCA calculations used in the comparison with TPS measurements have been excluded since both methods give a thermal conductivity of the same sample (3 sample excluded). In probability plots data from the TPS method has shown to be normal distributed but data from the SCA method does not display a normal distribution, see Appendix A. This is partly dependent on one outlier.

TPS and SCA values for the same samples are available for only three pairs. One sample was reported in /Sundberg et al. 2005b/ after correction for sericitisation and chloritisation. The mean difference between SCA and TPS for the three samples without any correction is 10.8%. On the basis of this difference it was decided to correct all SCA values by 10% i.e. a factor of 1.1. Although the number of samples on which this is based is very small, support for a difference of this order is given by comparing all TPS and SCA data for quartz monzodiorite from the Simpevarp subarea (Table 4-19). The SCA values are on average 12% lower than the TPS values.

Table 4-18. Two different distributions of thermal conductivity (W/(m·K)) for rock type quartz monzodiorite (501036), based on different methods together with the rock type model.

	TPS measurements	Calculations from mineral composition	Calculations from density loggings	Rock type model
Mean	2.74	2.41	–	2.69
Std dev	0.16	0.11	–	0.14
Number of samples	15	20	–	35
Comment	Data from three borehole intervals (< 5 m).	Comparable samples (three) indicate correction 10.8% (10% used).		TPS measurements and calculations from mineral composition (1.10·SCA) combined.

Table 4-19. Comparison of thermal conductivity (W/(m·K)) determined by different methods for rock type quartz monzodiorite (501036). Data from Simpevarp subarea only.

	Simpevarp subarea TPS	Simpevarp subarea SCA	Diff (SCA-TPS)/TPS
Mean	2.74	2.41	12%
Std dev	0.16	0.18	
No of samples	15	10	

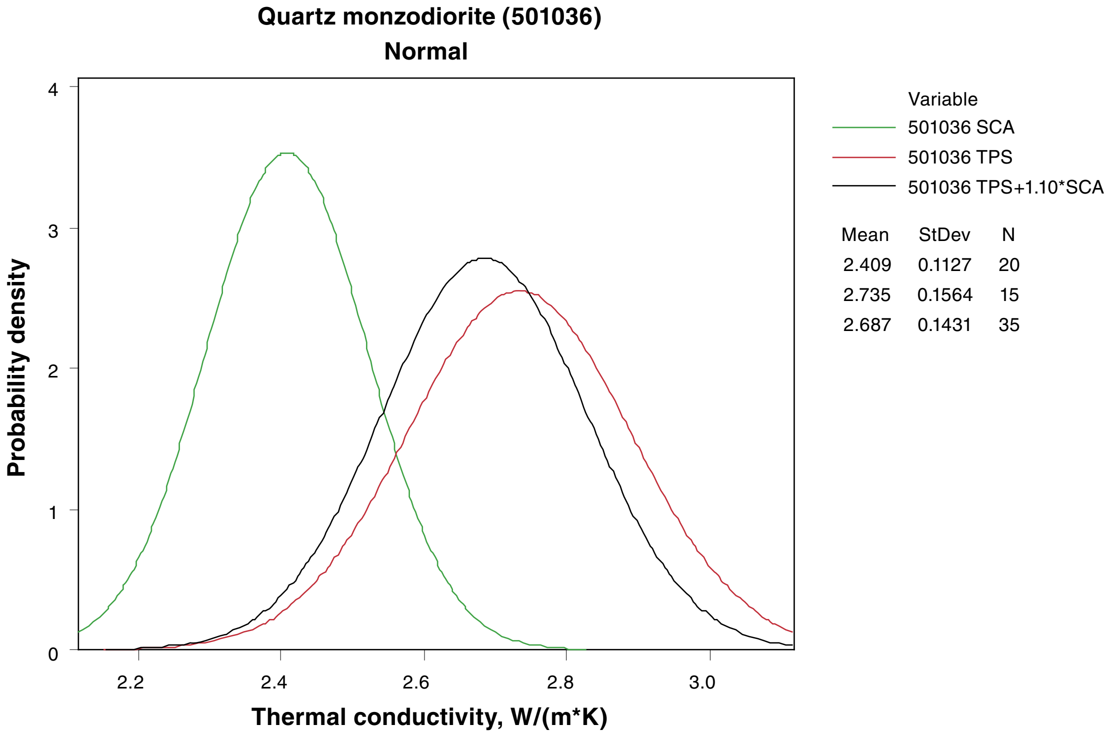

Figure 4-31. *PDF:s for calculated values (SCA), measured values (TPS), and rock type model (TPS+1.10·SCA) for rock type quartz monzodiorite (501036).*

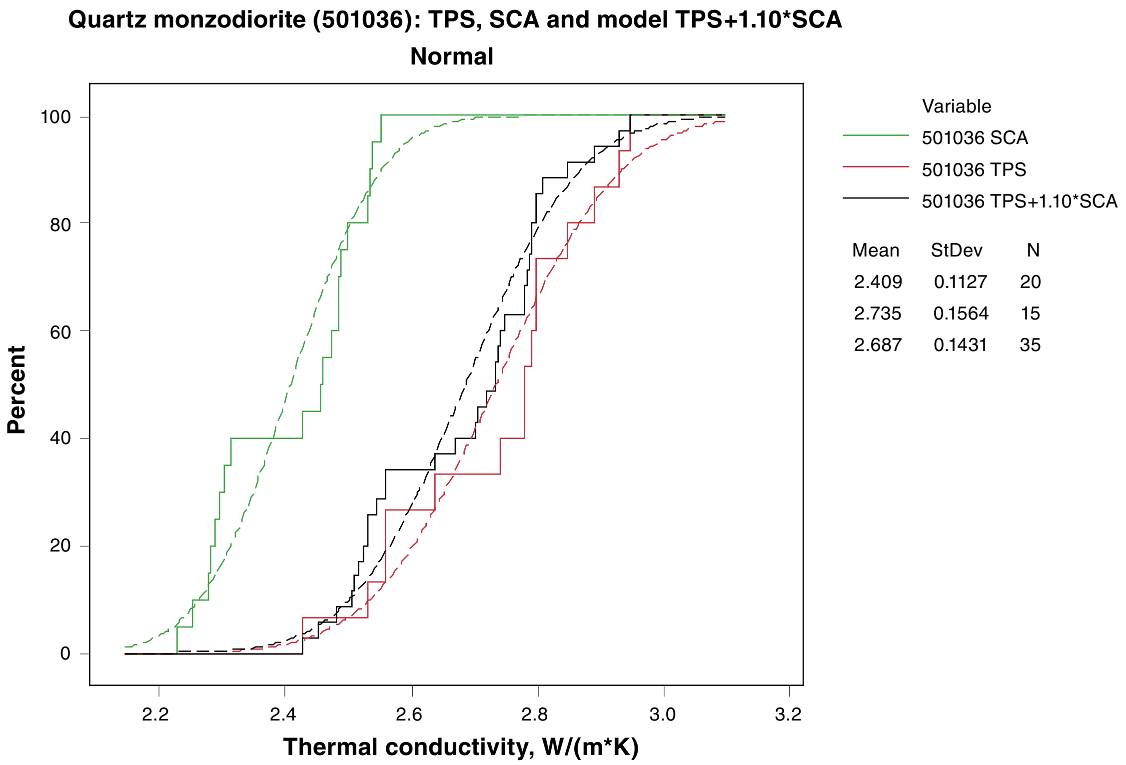

Figure 4-32. *Cumulative histogram of Quartz monzodiorite (501036) with data from two different methods and a rock type model where TPS and SCA data has been summed together.*

A rock type model of the thermal conductivity for rock type quartz monzodiorite (501036), used in the lithological domain modelling, is based on a combination of both TPS measurements and SCA calculations, see Table 4-18. The SCA calculations have been corrected by a factor of 1.10. The rock type model of TPS measurements and SCA calculations have been shown by probability plots not to follow a normal distribution Figure 4-26. Since the data may not be representative of the population a normal distribution cannot be rejected. Therefore, for modelling purposes the rock type model is assumed to have a normal distribution. In Simpevarp 1.2 the SCA data was also used in the rock type model but no correction was made to the data.

4.6.4 Fine-grained dioritoid (501030)

For rock type fine-grained dioritoid (501030) there are two sources to thermal conductivity data, SCA calculations and TPS measurements. Data from the two methods are summarised in Table 4-20. Models based on data from the different methods are presented in Figure 4-33 and Figure 4-34. As can be seen in the distribution functions in Figure 4-33 the two methods results in different mean values and variances. Table 4-21 shows that there is a difference in the distributions of SCA data between borehole and surface samples. Figure 4-34 presents empirical cumulative distribution functions with fitted models (normal distributions) of rock type fine-grained dioritoid (501030).

Table 4-20. Two different distributions of thermal conductivity (W/(m·K)) for rock type fine-grained dioritoid (501030) based on different methods together with the rock type model.

	TPS measurements	Calculations from mineral composition	Calculations from density loggings	Rock type model
Mean	2.79	2.40	–	2.72
Std dev	0.16	0.35	–	0.30
Number of samples	26	26	–	
Comment		Comparable sample indicate correction +10%		TPS measurements and calculations from mineral composition combined.

Table 4-21. Distributions of thermal conductivity data (W/(m·K)) from different methods for fine-grained dioritoid (501030) subdivided into borehole data and surface samples.

	SCA calculations		TPS measurements
	Surface samples	Borehole samples	Borehole samples
Mean	2.28	2.53	2.79
Std dev	0.24	0.40	0.16
Number of samples	13	13	26

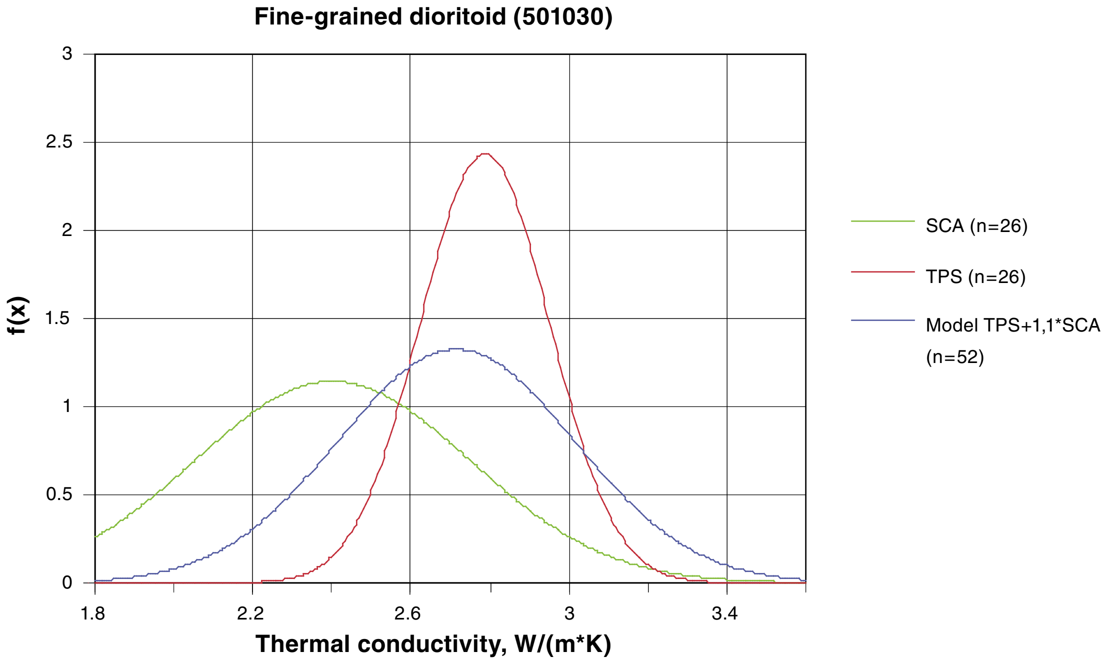

Figure 4-33. *PDF:s for calculated values (SCA) and measured values (TPS) based on rock type fine-grained dioritoid (501030). Data based on SCA are corrected with a factor 1.10 in the summarised rock type model.*

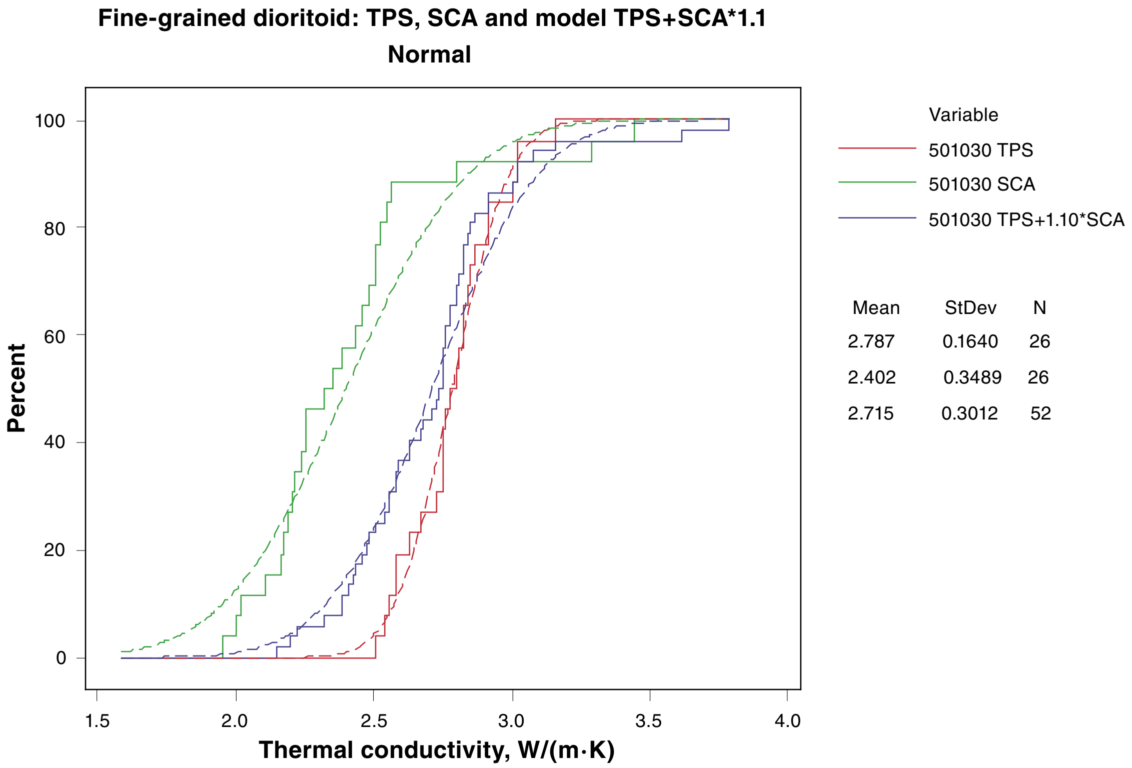

Figure 4-34. *Cumulative histogram of fine-grained dioritoid (501030) with data from two different methods and a rock type model where TPS and SCA data has been summed together.*

SCA calculations used in the comparison with TPS measurements have been excluded since both methods give a thermal conductivity of the same sample (5 samples excluded). Data from both the TPS method and the SCA methods has been shown in probability plots to be normal distributed, see Appendix A.

A rock type model of the thermal conductivity for the fine-grained dioritoid, used in the lithological domain modelling, has been constructed from a combination of both TPS measurements and SCA calculations. The SCA calculations has in this case been corrected with a factor 1.10 which in previous Section 4.4.3 has been shown as the difference between the two methods for this particular rock type. The model of TPS measurements and corrected SCA calculations has, using probability plots, been shown to be lognormal distributed rather than normal distributed but is still set to normal distributed, see Appendix A. (Excluding two outliers yields a better fit to a normal distribution. One outlier has been subsequently recognised as being incorrectly assigned to this rock type, see 4.4.2. The other outlier (KLX02: secup 553.2 m) has a corrected thermal conductivity values of 3.7, an unusually high value for this type of rock. A check of its mineral composition reveals a high chlorite content (17%), which can explain the high thermal conductivity for this sample.)

4.6.5 Other rock types (505102, 501033, 501058 and 511058)

For rock types other than Ävrö granite (501044), quartz monzodiorite (501036), and fine-grained dioritoid (501030), the extent of data is rather limited and in most cases only SCA calculations were available when modelling the different rock types. In Figure 4-35 empirical cumulative distribution functions of fine-grained diorite-gabbro (505102), diorite/gabbro (501033), granite (501058) and fine-grained granite (511058) is presented together with fitted models (normal distributions). Model properties of the above-mentioned rock types are presented in Table 4-22.

The mean thermal conductivities indicated by SCA calculations for the minor rock types are comparable to those presented for broadly similar rock types in /Sundberg 1988/. The mean SCA value for granite (501058) at 2.97 is somewhat lower than the mean value of Swedish granites, which was calculated as 3.47 /Sundberg 1988/. For pegmatite (501061) no data is available from the area of study. For this rock type data (mean and standard deviation) from /Sundberg 1988/ has been used.

4.6.6 All investigated tock types

In Table 4-22 the model properties for the different investigated rock types are summarized. Thermal conductivity calculated by the SCA method is available for all seven of these rock types. TPS measurements are available for four rock types, while thermal conductivity could be calculated from density for Ävrö granite (501044) only.

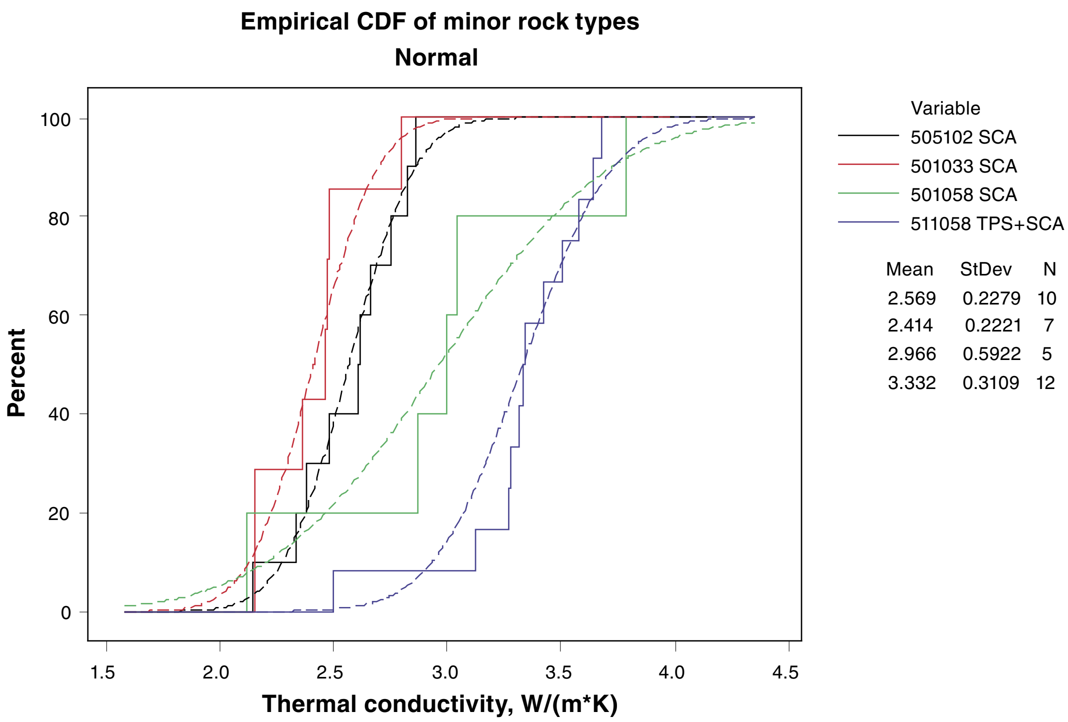

Figure 4-35. Cumulative histogram of fine-grained diorite-gabbro (505102), diorite/gabbro (501033), granite (501058) and fine-grained granite (501058). For the fine-grained granite (501058) data are from two different methods and a rock type model of summarised TPS and SCA data is illustrated. For the other three rock types (505102, 501033 and 501058), only SCA data is available.

Table 4-22. Model properties of thermal conductivity (W/(m·K)) from different methods and combinations divided by rock type. All rock type models (in bold) are based on normal (Gaussian) distributions (PDF:s).

Rock name (name code)	Samples	Mean	Std dev	Max	Min	No of samples	S1.2 – mean and std dev[1]	Comment
Ävrö granite	Therm. cond. from density logging	2.85	0.32[2]	3.74	1.84	22,711		Not used in model
(501044)	TPS	2.90	0.35	**3.76**	**2.16**	71		
	SCA	2.66	0.30	3.48	2.13	73		Not used in model
	Rock type model: TPS	**2.90**	**0.35**	**3.76**	**2.16**	**71**	2.79 (0.35)	
Quartz monzo-diorite	TPS	2.74	0.16	2.95	2.43	15		
(501036)	SCA	2.41	0.11	2.55	2.23	20		Adjusted by factor 1.1 in model
	Rock type model: 1.1·SCA+TPS	**2.69**	**0.14**	**2.95**	**2.43**	**35**	2.62 (0.28)	
Fine-grained dioritoid	TPS	2.79	0.16	3.16	2.51	26		
(501030)	SCA	2.40	0.35	3.45	1.96	26		Adjusted by factor 1.1 in model
	Rock type model: 1.1·SCA+TPS	**2.71**	**0.30**	**3.79**	**2.15**	**52**	2.72 (0.30)	

Rock name (name code)	Samples	Mean	Std dev	Max	Min	No of samples	S1.2 – mean and std dev[1]	Comment
Fine-grained granite	TPS	3.63	0.07	3.68	3.58	2		
(511058)	SCA	3.27	0.31	3.64	2.50	10		
	Rock type model: SCA+TPS	**3.33**	**0.31**	**3.68**	**2.50**	**12**	3.33 (0.34)	
Fine-grained diorite-gabbro								
(505102)	Rock type model: SCA	**2.57**	**0.23**	**2.87**	**2.15**	**10**	2.57 (0.23)	
Diorite/gabbro								
(501033)	Rock type model: SCA	**2.41**	**0.22**	**2.80**	**2.16**	**7**	2.46 (0.21)	
Granite								
(501058)	Rock type model: SCA	**2.97**	**0.59**	**3.79**	**2.12**[3]	**5**	2.59 (0.65)	
Pegmatite								
(501061)	Rock type model	**3.31**	**0.48**					Data from /Sundberg 1988/

[1] Site descriptive model Simpevarp version 1.2.
[2] The std dev of therm. cond. from density logging is partly a consequence of the restricted interval for the density vs thermal conductivity relationship.
[3] Sample with minimum value incorrectly assigned to rock type 501058 in SICADA.

4.7 Spatial variability

4.7.1 Spatial variability in thermal conductivity from measurements

In order to estimate thermal conductivity at a scale larger than the measurement scale, upscaling from TPS scale (cm) can be performed by calculation of the geometric mean for samples in groups over a certain limited distance. This method is treated in /Sundberg et al. 2005a/. However, data adequate for this purpose is not available from Laxemar.

4.7.2 Spatial variability in thermal conductivity from density loggings

There are three main causes for the spatial variability of thermal conductivity at the domain level; (1) small scale variability between minerals, (2) spatial variability within each rock type, and (3) variability between the different rock types making up the domain.

The second type of variability involves spatial variability within each rock type that cannot be explained by small scale variations. This is believed to be especially important for the rock type Ävrö granite, where this (spatial) variability is large. Variability within a rock type is largely the result of rock-formation processes but may also be a consequence of the system of classifying the rock types. This variability cannot be reduced but the uncertainty of the variability may be reduced. This is achieved by collecting a large number of samples at varying distances form each other, so that reliable variograms can be created.

Spatial variability of thermal conductivity within rock types has only been studied for rock type Ävrö granite (501044), where density loggings could be used. For other rock types it was not possible to study the spatial variability because of too few measurements and a lack of a reliable relationship between density and thermal conductivity.

Variograms of thermal conductivity for Ävrö granite (501044) in four different boreholes (KLX01, KLX02, KLX03 and KLX04) are illustrated in Figure 4-36 to Figure 4-39 at various scales. Several different correlation lengths (ranges) can be identified depending on scale. Variograms for the four different boreholes show some general tendencies:

- Strong correlation at the metre scale is obvious in all boreholes. Between approximately 25% and 80% of the total variance in data can be explained by variability up to distances of 1–1.5 m. Much of this variability is produced by the random noise in density logging measurements. The correlation up to 0.5 m is to some extent affected by the filtering of logging data, and possibly also by overlapping measurement volumes due to the density logging technique.
- Correlation up to about 5–15 m is apparent in several of the boreholes, for example, KLX04.
- Weak correlation exists up to between 100 and 300 m, varying somewhat from boreholes to borehole. The variability at this scale is often larger than the total variability in data.

4.7.3 Spatial variability of rock types

To examine the spatial variability of different rock types several indicator variograms have been made and are presented in Appendix C. Data has been processed for domains RSMA and RSMD. The evaluation of spatial variability of rock types is not complete, and in this model version the indicator variograms have not been used.

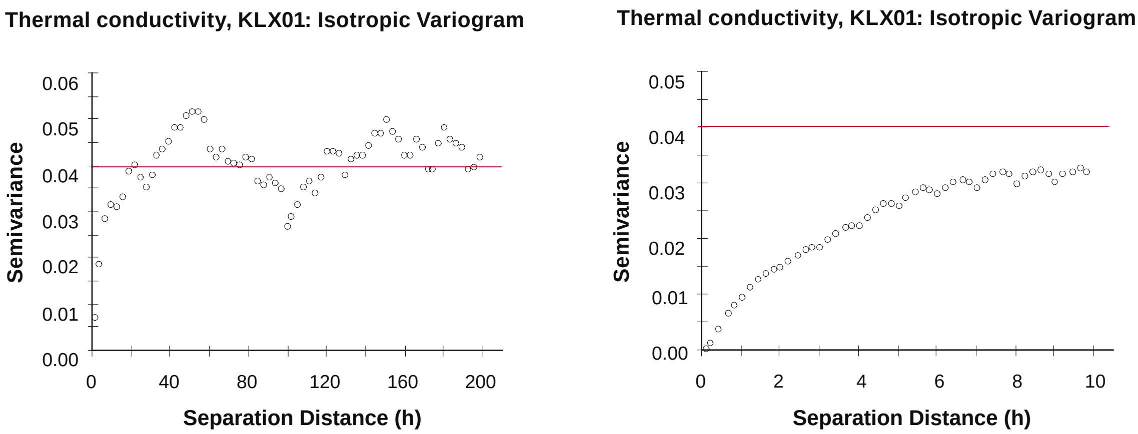

Figure 4-36. *Variogram of thermal conductivity for Ävrö granite (501044) in KLX01, estimated from density logging; 0–100 m and 0–10 m separation distance. The straight line indicates the total variance in data. An exponential model has been fitted to the data.*

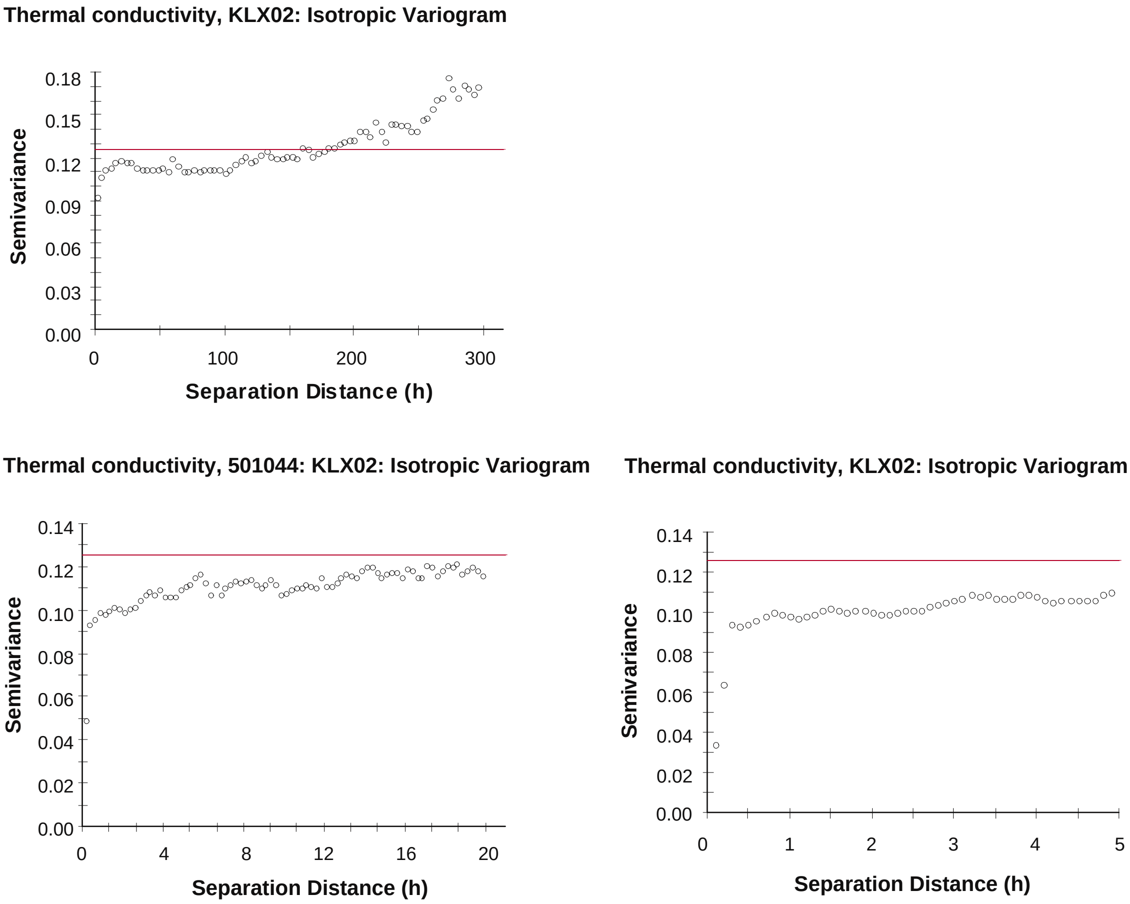

Figure 4-37. *Variogram of thermal conductivity for Ävrö granite (501044) in KLX02, estimated from density logging; 0–350 m and 0–20 m separation distance. The straight line indicates the total variance in data.*

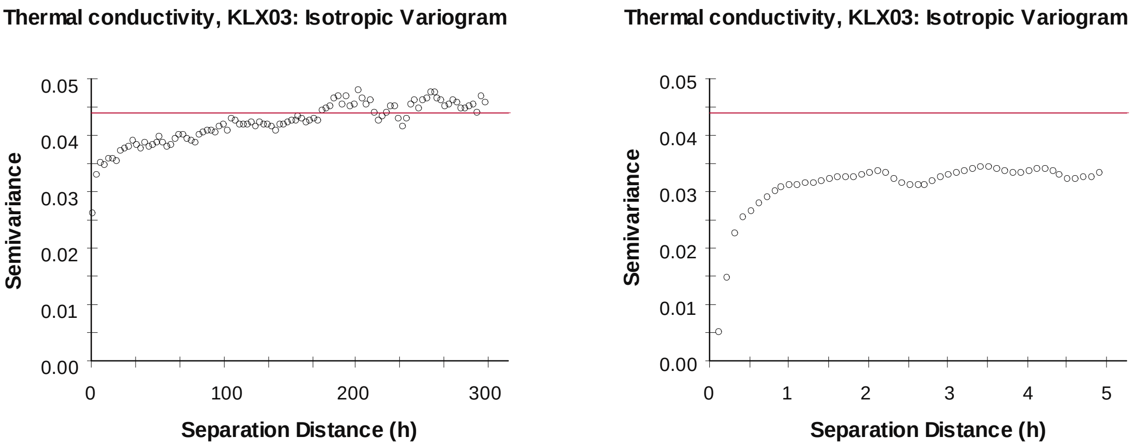

Figure 4-38. *Variogram of thermal conductivity for Ävrö granite (501044) in KLX03, estimated from density logging; 0–20 m and 0–5 m separation distance. The straight line indicates the total variance in data. An exponential model has been fitted to the data in the figure on the right hand side.*

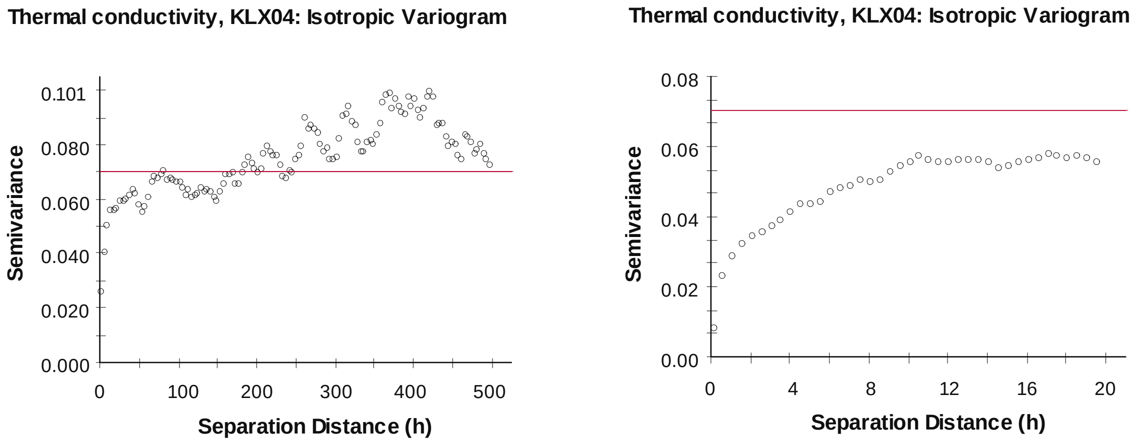

Figure 4-39. *Variogram of thermal conductivity for Ävrö granite (501044) in KLX04, estimated from density logging; 0–100 m and 0–20 m separation distance. The straight line indicates the total variance in data. An exponential model has been fitted to the data.*

4.8 Anisotropy

Measurements to asses anisotropy in thermal conductivity and heat capacity for samples within the Laxemar subarea have not been carried out as part of the current data freeze. Nor has anisotropy been considered in the domain modelling. Anisotropic effects may result from the presence of subordinate rock types occurring as dykes of significant extension, consisting of a rock type with different thermal characteristics. It may also arise from structural foliations or lineations in dominant rock types.

With the exception for the rocks of the major deformation zones, the rocks in the Laxemar subarea are generally isotropic /Nilsson et al. 2004/. Only locally is a weak foliation developed. When observed in the Ävrö granite, this foliation is obvious in the matrix while orientation of megacrysts is either only weakly developed or absent altogether. Magnetic anisotropy data indicate a regional rock fabric striking west to west-northwest, parallel to the major lithological boundaries /Mattsson et al. 2004/. A weaker secondary fabric (N-S to NE-SW) occur in all rock types apart from fine, medium and coarse-grained granites. The degree of anisotropy, however, is generally moderate to low /Mattsson et al. 2004/.

The effect on thermal properties of structure and foliation in dominant rock types has not been investigated in this study, but is assumed to be small. Activities to verify or disprove this assumption are being considered for future investigations.

Large-scale anisotropy may be present as a result of the preferential orientation of subordinate rock types. Fine to medium-grained granite, which makes up approximately 3% of the total rock volume in the boreholes of the Laxemar subarea investigated in this study, occurs as minor bodies and dikes throughout the Laxemar subarea /Nilsson et al. 2004/. The dikes strike predominantly NE-SW while their dip varies from vertical to shallow /SKB 2006/. Other rock types occurring as dykes are pegmatite and fine-grained diorite to gabbro, the latter also occurring as minor bodies and enclaves. A preferred orientation has not been reported for these rock types, although such a feature cannot be excluded as of present.

Modelling of this large-scale anisotropy has not been carried out for the Laxemar subarea, but some conclusions can nevertheless be made. Given that the fine-grained granite has higher thermal conductivities than the rock which it intrudes, namely Ävrö granite, this would imply that in the direction parallel to the dikes, i.e. NE-SW, thermal conductivity would be higher than in other directions. However, because of the relatively minor importance of fine-grained granite the effects on thermal conductivity are considered to be small.

4.9 Heat capacity

4.9.1 Method

Heat capacity has been determined indirectly from measurements with the TPS (Transient Plane Source) method. No direct laboratory measurements of the heat capacity have been carried out, but the volumetric heat capacity has been calculated from conductivity and diffusivity measurements performed with the TPS method. For method description see Section 4.3.1.

4.9.2 Results: rock type models

In Table 4-23 the results from heat capacity determinations for different rock types are summarised. Determination of heat capacity has been performed on the same samples as used for measurement of thermal conductivity, cf Section 4.3. Therefore the same problem concerning representativeness of the rock mass exists. Observe that samples from rock type Ävrö granite (501044) are collected from the Simpevarp subarea /Adl-Zarrabi 2004abcd/, the Laxemar subarea /Adl-Zarrabi 2004ef/ and the Äspö HRL /Sundberg and Gabrielsson 1999, Sundberg 2002, Sundberg et al. 2005a/. Samples from rock type fine-grained dioritoid (501030) and quartz monzodiorite (501036) all come from the Simpevarp subarea /Adl-Zarrabi, 2004abcd/. Some of the samples are spatially located in groups with approximately 2–5 samples in each group. Rock type models of heat capacity have been produced from the results in Table 4-23. Probability plots of heat capacity indicate that the normal distribution models used in domain modelling are appropriate for Ävrö granite and fine-grained dioritoid (Figure 4-40). A lognormal distribution model gives a slightly better fit than a normal distribution model for the quartz monzodiorite data.

4.9.3 Temperature dependence

The temperature dependence of heat capacity has been investigated by measurements for the three rock types Ävrö granite (501044), fine-grained dioritoid (501030) and quartz monzodiorite (501036), at three different temperatures (20, 50 and 80°C) /Adl-Zarrabi 2004abef /. For rock type Ävrö granite (501044), thermal conductivity has been measured on four samples at four different temperatures (25, 40, 60 and 80°C) /Sundberg 2002/. The temperature dependence of each sample is illustrated in Figure 4-41 to Figure 4-44 and summarised per rock type in Table 4-24. Heat capacity increases with increasing temperature.

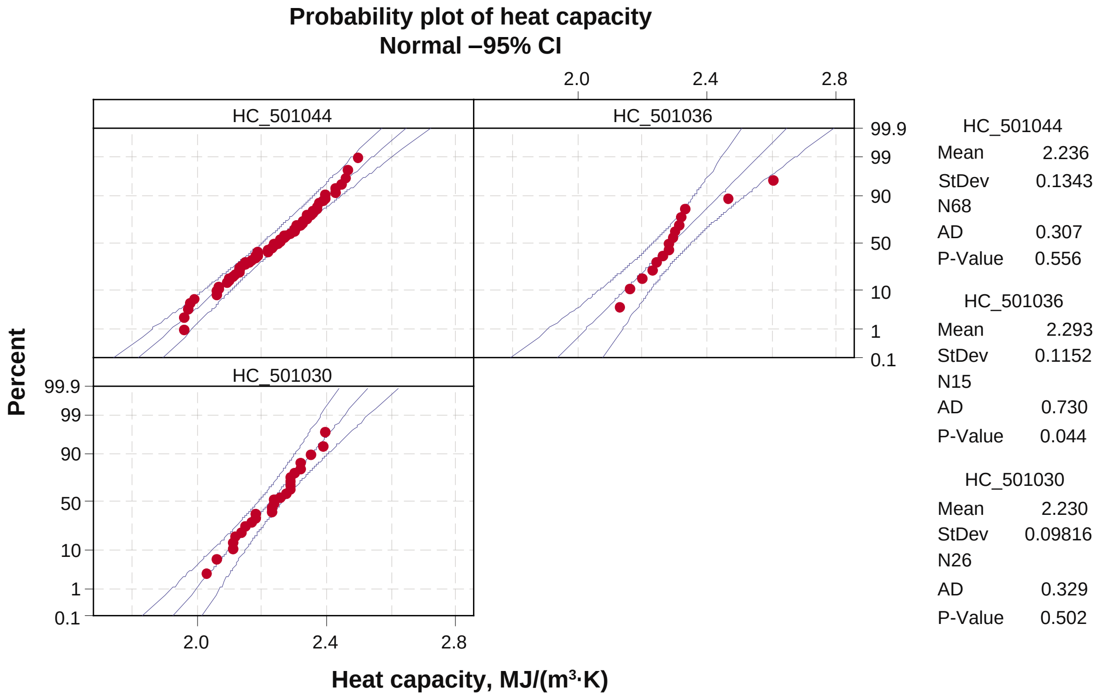

Figure 4-40. *Probability plots (normal distributions) of heat capacity for different rock types.*

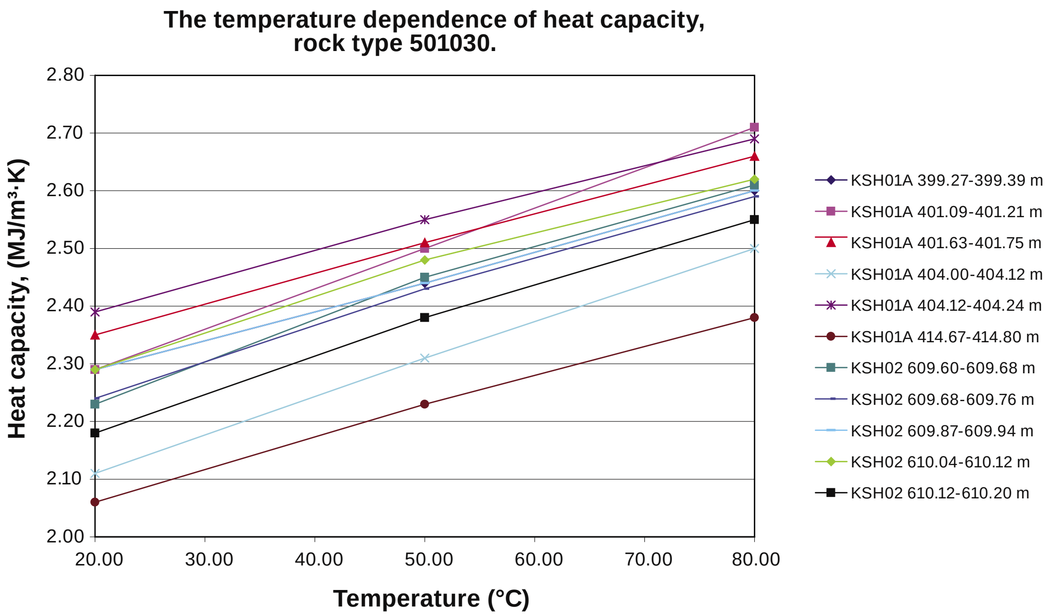

Figure 4-41. *Temperature dependence of heat capacity, rock type fine-grained dioritoid (501030).*

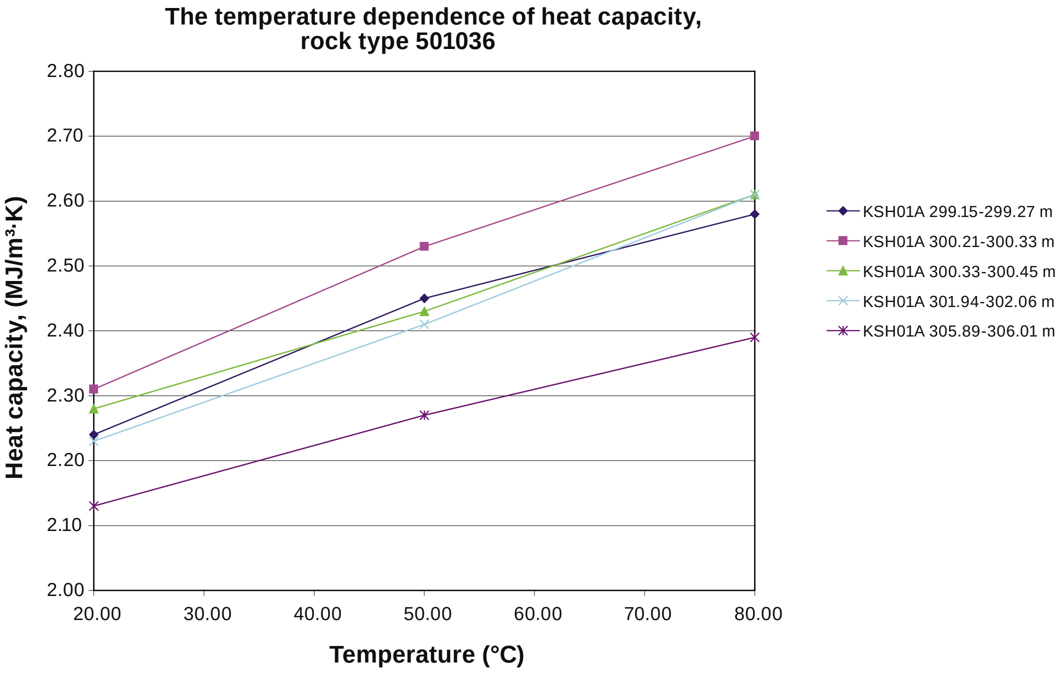

Figure 4-42. *Temperature dependence of heat capacity, rock type quartz monzodiorite (501036).*

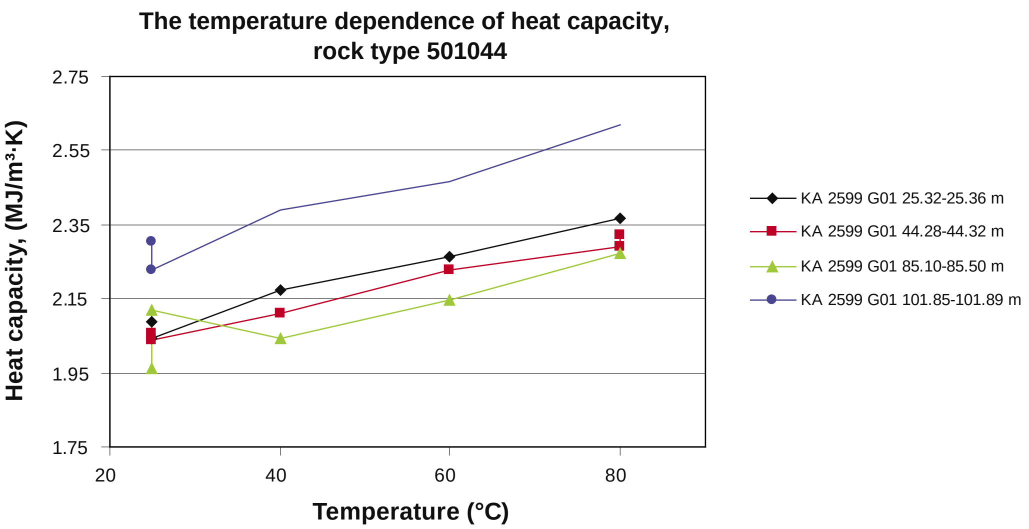

Figure 4-43. *Temperature dependence of heat capacity, rock type Ävrö granite (501044).*

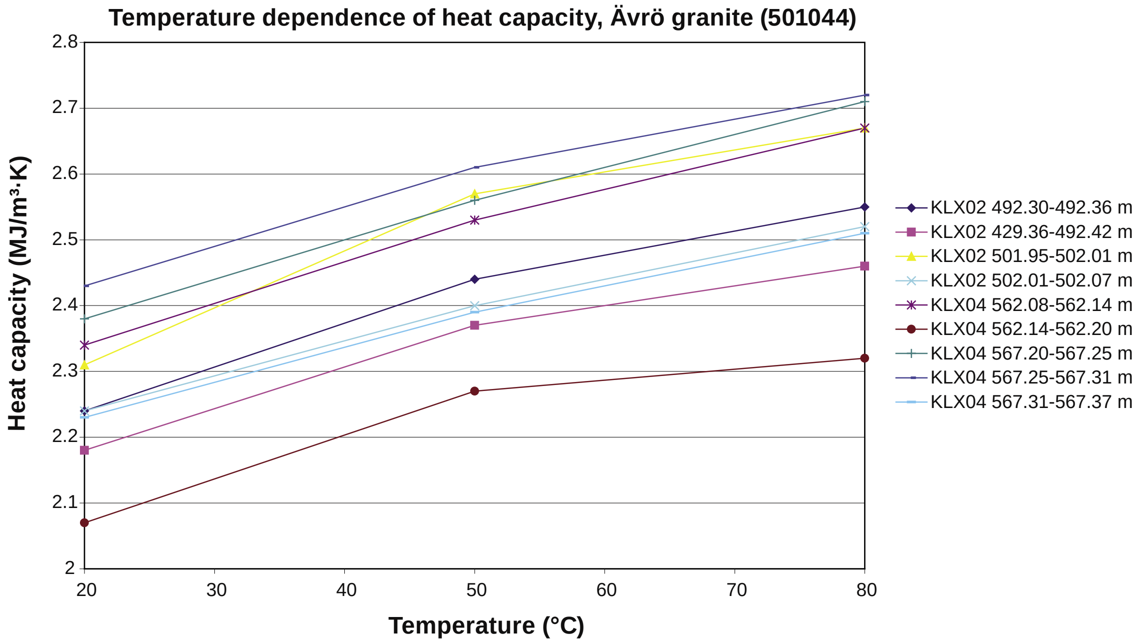

Figure 4-44. *Temperature dependence of heat capacity, rock type Ävrö granite (501044).*

Table 4-23. Determined heat capacity (MJ/(m³·K)) of samples from different rock types, using the TPS method. Samples are from boreholes KAV01, KSH01A, KSH02, KAV04a, KLX02 and KLX04 (Simpevarp and Laxemar subareas) together with borehole KA2599G01 (Äspö HRL) and boreholes from the prototype repository tunnel (Äspö HRL).

Rock name (sample location)	Mean	Std dev	Number of samples
Fine-grained dioritoid, 501030 (borehole KSH01A and KSH02)	2.23	0.10	26
Quartz monzodiorite, 501036 (borehole KSH01A and KAV04A)	2.29	0.13	15
Ävrö granite, 501044 (borehole KAV01, KAV04A, KLX02, KLX04, KA2599G01 and Äspö HRL prototype tunnel)	2.24	0.13	68

Table 4-24. Determined temperature dependence of heat capacity (per 100°C temperature increase) on samples from different rock types in boreholes KSH01A and KSH02 (Simpevarp subarea), KLX02 and KLX04 (Laxemar subarea), and KA2599G01 (Äspö). The mean of the temperature dependence is estimated by linear regression.

Rock name (name code) (sample location)	Mean	Std dev	Number of samples
Fine-grained dioritoid (501030) (boreholes KSH01A and KSH02)	25.6%	3.51%	11
Quartz monzodiorite (501036) (borehole KSH01A)	25.3%	3.30%	5
Ävrö granite (501044) (boreholes KA2599G01, KLX02 and KLX04)	25.1%	5.74%	13

4.10 Coefficient of thermal expansion

The coefficient of thermal expansion has been measured on samples from the Simpevarp and Laxemar areas /Åkesson 2004abcdef/. Samples from six different boreholes (KSH01A, KSH02, KAV01, KAV04A, KLX02 and KLX04) have been investigated. The results grouped according to rock type are presented in Table 4-25. The mean values of measured thermal expansion for the different rock types varies between $6.9 \cdot 10^{-6}$ and $8.2 \cdot 10^{-6}$ m/(m·K).

Earlier measurements of thermal expansion made at the Äspö HRL were performed on rocks subsequently reclassified as Ävrö granite. These results, summarised in /Sundberg et al. 2005b/, show slightly higher thermal expansion coefficients than more recent measurements on Ävrö granite. However, the laboratories and methods were not the same as for the results reported above.

Table 4-25. Measured coefficient of thermal expansion (m/(m·K)) on samples with different rock types from boreholes KSH01A, KSH02, KAV01, KAV04A, KLX02 and KLX04 at the Simpevarp and Laxemar sites (temperature interval: 20–80°C).

Rock type	Mean value	Std dev	Min	Max	Number of samples
Fine-grained dioritoid (501030) (boreholes KSH1A and KSH02)	$6.9 \cdot 10^{-6}$	$1.5 \cdot 10^{-6}$	$4.6 \cdot 10^{-6}$	$9.9 \cdot 10^{-6}$	17
Quartz monzonite to monzodiorite (501036) (boreholes KSH01A and KAV04A)	$8.2 \cdot 10^{-6}$	$1.3 \cdot 10^{-6}$	$5.8 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	14
Granite to quartz monzodiorite (501044) (boreholes KLX02, KLX04, KAV01 and KAV04A)	$7.2 \cdot 10^{-6}$	$1.8 \cdot 10^{-6}$	$4.3 \cdot 10^{-6}$	$1.1 \cdot 10^{-5}$	41

4.11 In situ temperature

4.11.1 Method

Temperature and vertical temperature gradient profiles have been investigated for the boreholes KLX01, KLX02, KLX03, KLX04 and KAV04. The temperature was measured by fluid temperature loggings using a logging interval of 1 dm. Measured temperatures have been filtered for all investigated boreholes except KLX02. Temperature and temperature gradient have been plotted against elevation in the diagrams below, Figure 4-45 to Figure 4-50.

For all series with temperature measurements, equations were also fitted, to be used for other applications. For KLX02 three temperature loggings have been made, in 1993, 2002 and 2003, and one equation was produced for each of the series. For KLX02 year 2002, the logging interval was 2 cm, giving too many temperature values for the calculation program to handle. For this series, every second value was excluded when calculating an equation. Both linear, second degree and third degree equations were evaluated. The linear equations where considered to be satisfactory, since higher degree equations did not give a markedly larger correspondence.

Vertical thermal gradients were calculated for the midpoint of a 9 m interval of the borehole length. This means that, since the logging interval is 1 dm, 91 temperature values were used for each gradient value, If loggings have been made using other intervals (e.g. KLX02, 2002), the equation has been corrected accordingly. The gradients were calculated according to Equation 4-3.

$$Gradient = \frac{1000(n\Sigma zT - \Sigma z\Sigma T)}{n\Sigma z^2 - (\Sigma z)^2} \quad \text{Equation 4-3}$$

Parameter z is the depth co-ordinate, elevation (m) T is the measured temperature (°C), and n is the number of temperature measurements in the interval. Temperature gradients were also calculated for vertical distances of several hundred metres, but only for those parts of the borehole along which large temperature gradient anomalies are absent.

4.11.2 Results

The results from the temperature loggings, the equations for the temperature and the calculated gradients are presented in Figure 4-45 to Figure 4-50**.** Figure 4-45 illustrates a summary of all investigated boreholes and Figure 4-46 to Figure 4-50 the boreholes separately. For KLX02, measurements and calculations from three different occasions are illustrated in the figures. The y-axis in the figures illustrates depth below sea level (not the borehole length). In Table 4-26 the elevation (metres above sea level) for the start points for the boreholes are presented. The differences depend on the ground elevation above sea level.

The filtered temperatures in each borehole seem to be almost linear with depth. In Table 4-27 the temperatures at different depths are presented for the four investigated boreholes in the Laxemar subarea, and the mean temperature at different depths is calculated. In this calculation only the latest value for KLX02 is used and the other ones are excluded. In the same table, the approximate inclinations for the boreholes are also presented.

Times for core drillings and fluid temperature loggings for three of the boreholes are given in Table 4-28. The times between core drilling and temperature logging are about 3 weeks for KLX03, 16 weeks for KLX04 and 4 weeks for KAV04A. The relatively short period between the drilling activity and temperature logging might result in a disturbance of the logging results due to the borehole not being stabilised. The drilling activity increases the temperature in the borehole but a temperature decrease probably occurs due to the added drilling fluid. Moreover, a temperature equalisation occurs in the borehole when the drilling fluid is transported in the borehole. Also errors associated with calibration of the temperature sensors have recently been recognized. Thus, there are potential errors in the loggings and this is indicated by the noted difference in temperature for the same borehole logged on different occasions. However, this difference in temperature is relatively small for a specified depth but the influence on the design of a repository may be significant.

The angle for borehole KLX01 varies between 85° and 87°. The gradient has also been calculated for the interval –200 to –600 m. This resulted in a gradient of about 16°C/km.

The angle for borehole KLX02 decreases from 85° close to the surface, to 83° at –1,000 m and to 82° at –1,400 m. Gradients for the three different loggings (1993, 2002 and 2003) have been calculated and are shown in Figure 4-47. There are large oscillations in all three of the gradients and they do not follow each other. For the gradient calculated from data for 2003, the oscillations are smaller than for the other two. The mean gradient for the interval –300 to –700 m is about 15°C/km for all three data sets. From results from 1993, the gradient for the interval –800 to –1,200 m is about 16°C/km.

For borehole KLX03 the angle increases from 75° at –100 m to 77° at –800 m. The calculated gradient for the interval –350 to –650 m is 17°C/km.

The angle for borehole KLX04 varies between 82 and 85°. The gradient is about 19°C/km for the interval –400 to –800 m.

From –100 m to –600 m the angle for borehole KAV04A varies between 85° and 86°, below which it decreases slightly. The gradient is almost 18°C/km for the interval –500 to –800 m.

The difference between the temperature at different occasions and in different boreholes is sometimes rather large, see Figure 4-45. This is discussed further in Section 6.3.

Table 4-26. Ground level for the start points of boreholes within the Laxemar and Simpevarp subareas.

Borehole	Elevation (metres above sea level)
KLX01	16.8
KLX02	18.4
KLX03	ca 18
KLX04	ca 24
KAV04A	ca 10

Table 4-27. Temperature (°C) for the four investigated boreholes in the Laxemar subarea, at different depths below ground surface. For KLX02, measurements are made at three different occasions, and data have not been filtered and resampled. Inclination of the boreholes is also indicated.

Borehole	Temperature at 400 m below ground level	Temperature at 500 m below ground level	Temperature at 600 m below ground level	Inclination (°)
KLX01	13.4	15.1	16.6	85–87
KLX02, 1993	12.3	13.8	15.3	82–85
KLX02, 2002	12.7	14.2	15.7	83–85
KLX02, 2003	13.1	14.5	16.1	83–85
KLX03	11.1	12.8	14.5	75–77
KLX04	11.4	13.2	15.1	82–85
Mean	12.3	13.9	15.6	(For calculation of mean temperature, only the latest value for KLX02 is used)

Table 4-28. Dates for core drilling, and fluid temperature and resistivity loggings for the boreholes KLX03, KLX04 and KAV04A.

Borehole	Core drilling Start time	Core drilling Stop time	Fluid temperature and resistivity logging
KLX03	28 May 2004	7 Sept 2004	30 Sept 2004
KLX04	13 March 2004	28 June 2004	20 Oct 2004
KAV04A	10 Dec 2003	3 May 2004	2 June 2004

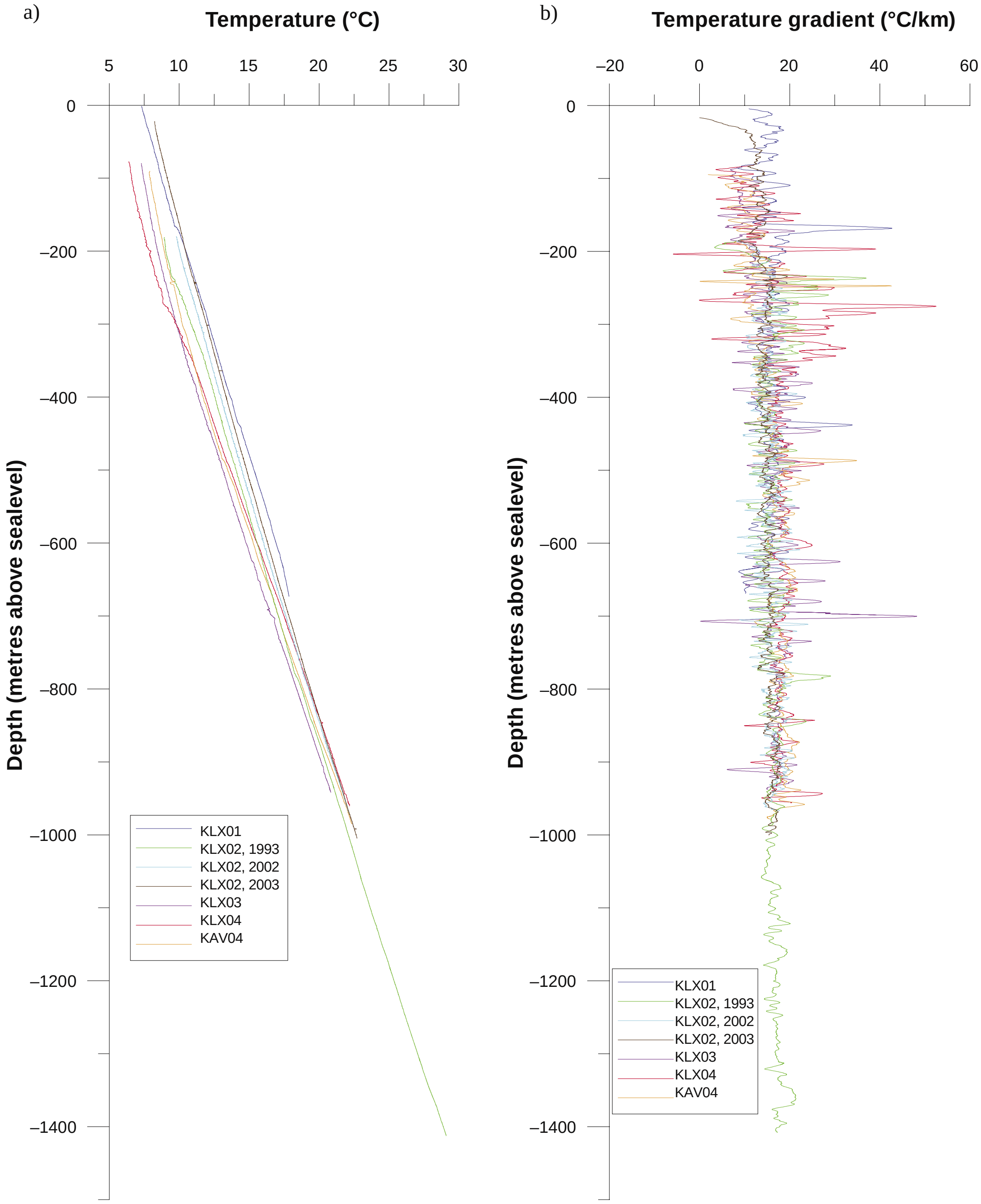

Figure 4-45. *Temperature (a) and vertical temperature gradients in boreholes (b) for four boreholes at Laxemar and one at Ävrö. The temperature gradient is calculated for nine metre intervals.*

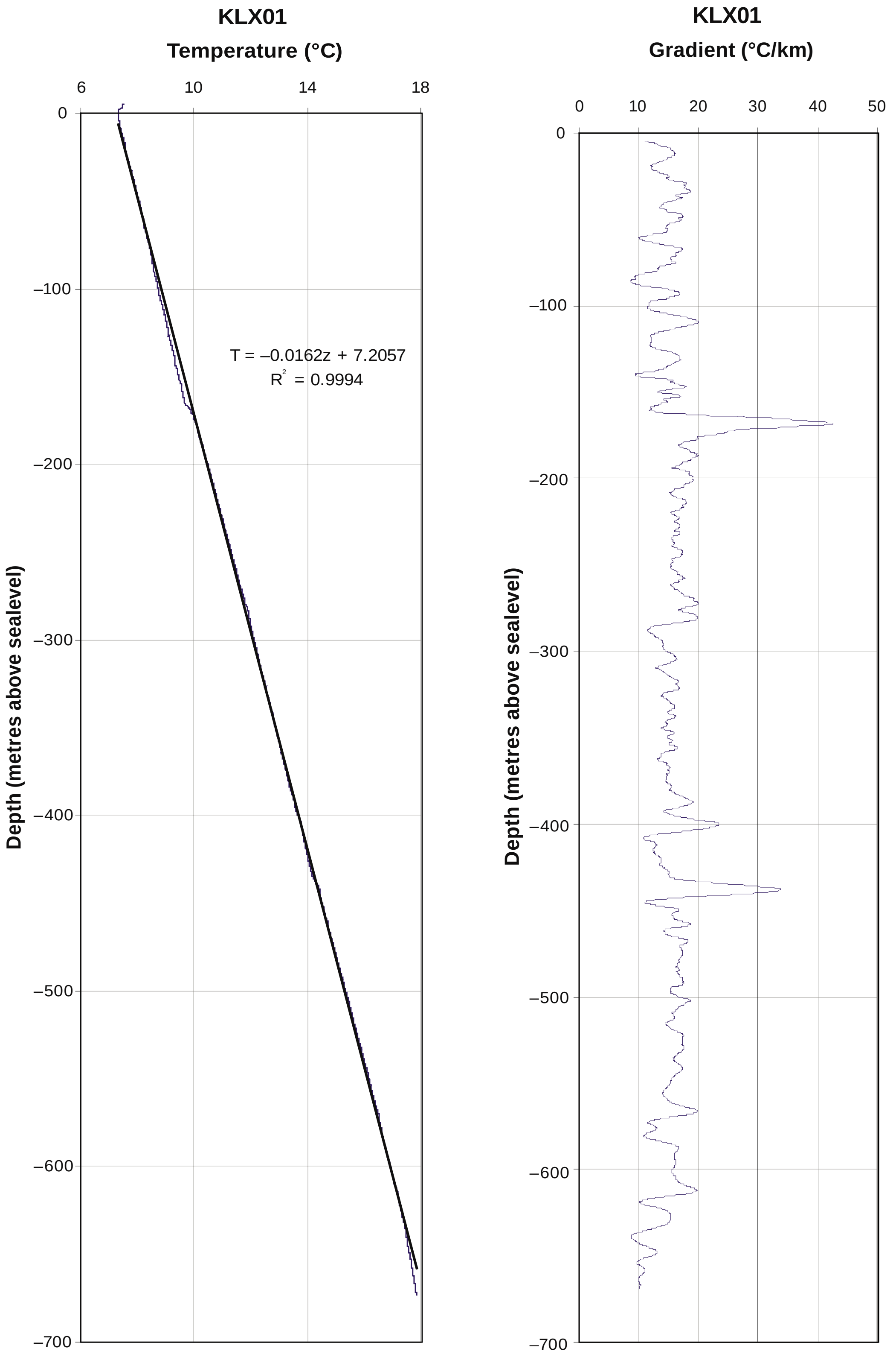

Figure 4-46. *Temperature (a) and vertical gradient (b) for KLX01, Laxemar subarea. The gradient is calculated for nine metre intervals.*

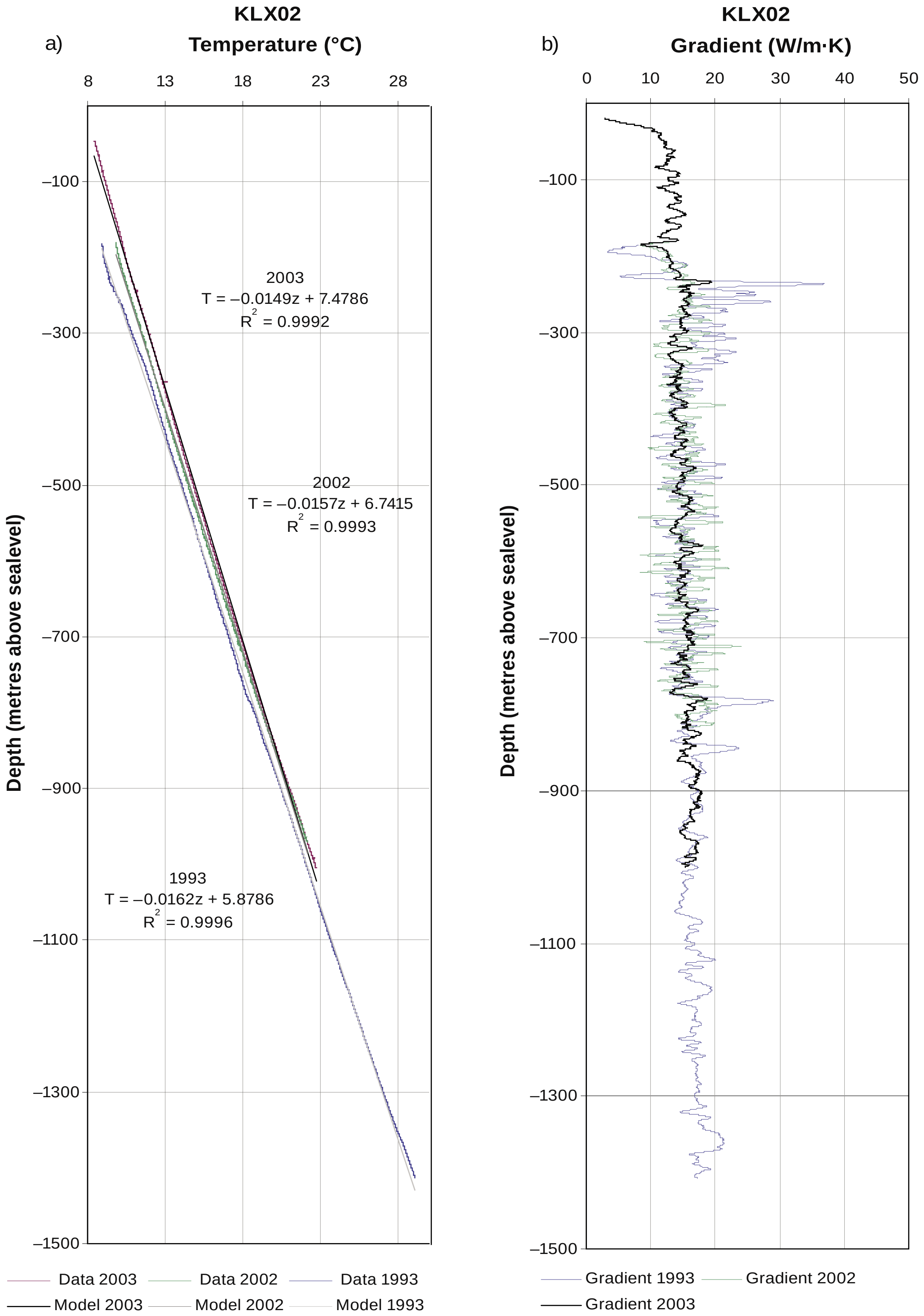

Figure 4-47. *Temperature (a) and vertical gradient (b) for KLX02, Laxemar subarea. The gradient is calculated for nine metre intervals.*

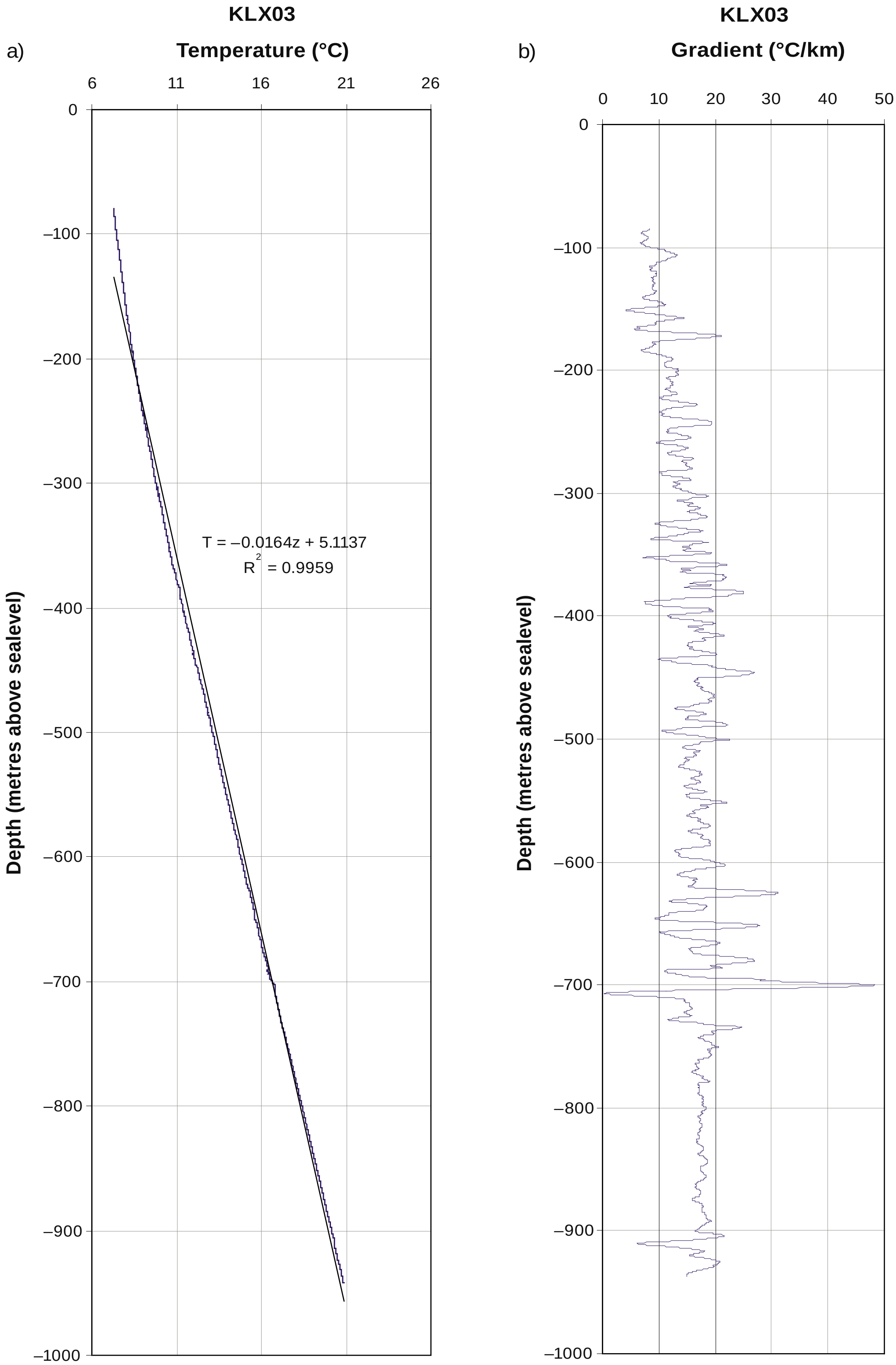

Figure 4-48. *Temperature (a) and vertical gradient (b) for KLX03, Laxemar subarea. The gradient is calculated for nine metre intervals.*

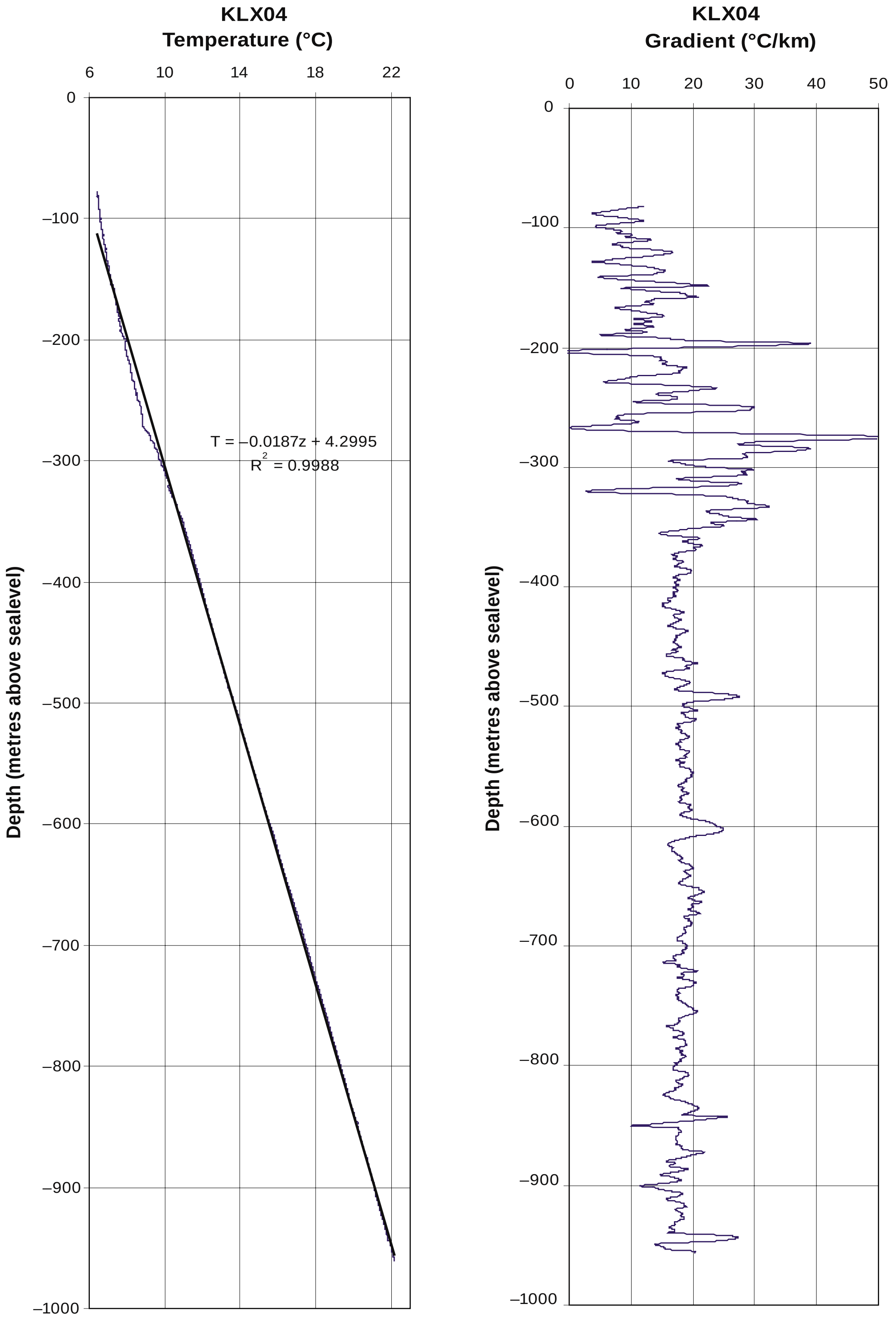

Figure 4-49. *Temperature (a) and vertical gradient (b) for KLX04, Laxemar subarea. The gradient is calculated for nine metre intervals.*

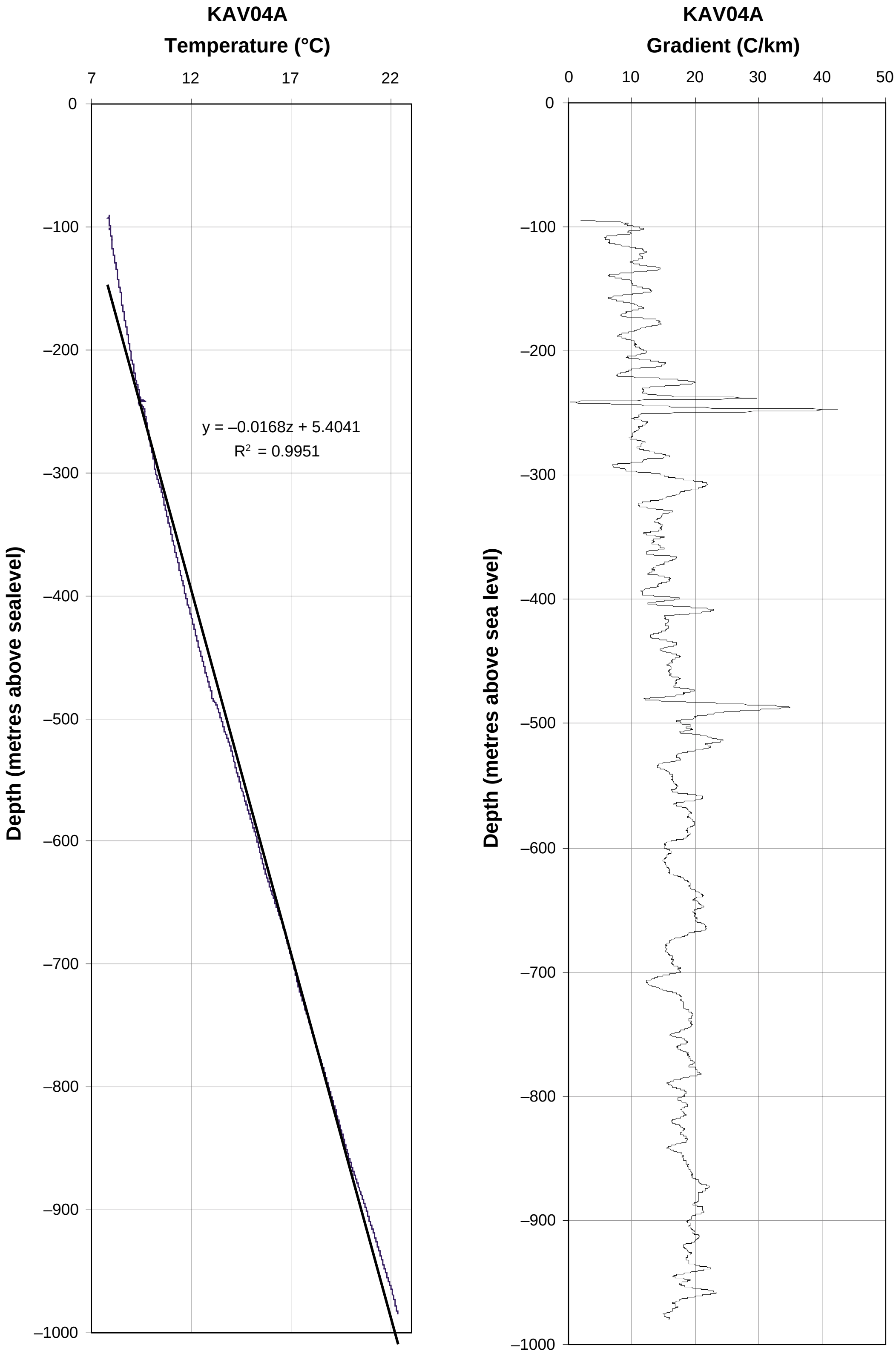

Figure 4-50. *Temperature (a) and vertical gradient (b) for KAV04, Simpevarp subarea. The gradient calculated for nine metre intervals.*

For some of the boreholes, difference flow loggings were performed in order to determine the transmissivity and the hydraulic head in the borehole sections and fractures in the borehole. To do this, the Posiva flow log (PFL) is used. The equipment for this includes a temperature sensor with the temperature being measured every 5th m. These results are presented in /Rouhiainen et al. 2005/. In Figure 4-51 temperature results from the fluid temperature and resistivity logging and from the difference flow logging (downwards, without pumping) for borehole KLX03 are shown for comparison. According to /Rouhiainen et al. 2005/ the accuracy for the temperature sensor is 0.1°C.

The temperature measurements made in KLX03 in connection with the Posiva flow log gives the temperature 12.8°C at 400 m below ground level, 14.5°C at 500 m below ground level and 16.1°C at 600 m below ground level. This is about 1.5°C higher than the results from the fluid temperature logging. The accuracy for the fluid temperature logging is low because of errors associated with measurement and calibration, see further Section 6.3. The difference might also be partly due to the longer time elapsed between drilling and PFL logging (5–6 Nov, 2004). The fluid temperature logging, on the other hand, was carried out on 30 Sept, 2004, only a few weeks after drilling was terminated. The temperature conditions in the borehole may not have stabilised fully by then.

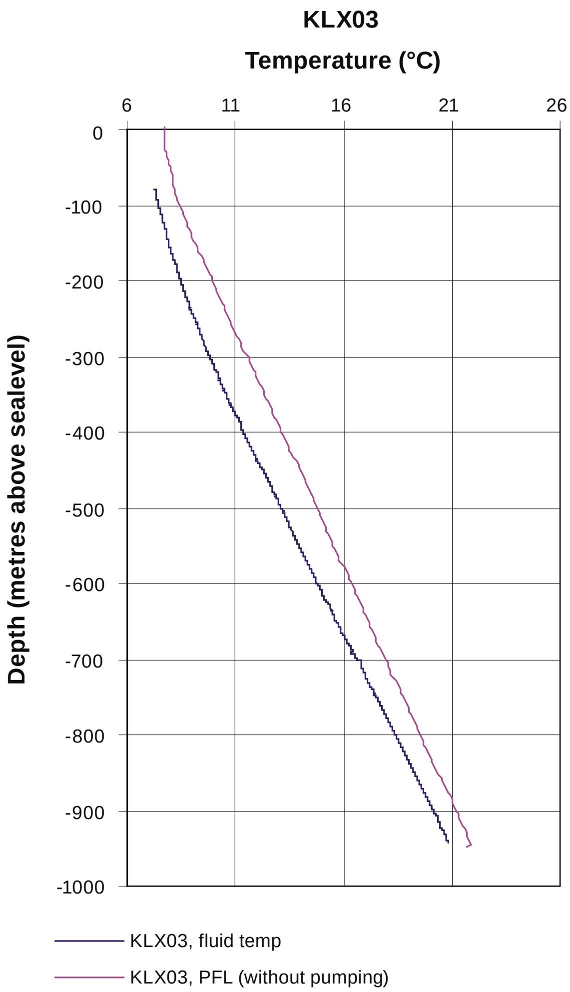

Figure 4-51. *Temperature measured according to two different methods for KLX03. The temperature has been measured by fluid temperature and resistivity logging and by PFL-measurement.*

5 Thermal modelling of lithological domains

5.1 Modelling assumptions and input from other disciplines

5.1.1 Geological model

The rock domain model from the Laxemar site descriptive model version 1.2 forms the geometrical base for the thermal model and is described briefly in Section 4.2 and in greater detail in /SKB 2006/. The Laxemar subarea west of the plastic deformation zones (domains RSMP01 and RSMP02) is characterised by five lithological domains as described in Table 5-1 and illustrated in Figure 4-2.

The geological boremap log of the boreholes, showing the distribution of dominant and subordinate rock types, together with a lithological domain classification of borehole intervals (Table 5-2) has, after modification, been used as input to the thermal modelling. The available data is considered to be representative of the domains, allowing the numerical subscript in domain names to be omitted.

Table 5-1. Nomenclature of rock domains referred to in this report.

Domain	Description
RSMA	Dominated by Ävrö granite
RSMBA	Mixture of Ävrö granite and fine-grained dioritoid
RSMD	Dominated by quartz monzodiorite
RSME	Dominated by diorite/gabbro
RSMM	Mixed zone with large fraction of diorite/gabbro

Table 5-2. Boreholes classified by domain /SKB 2006/.

Domain	Borehole	Comment
RSMA	KLX01 0–1,078 m	Based on subdomain RSMA01
	KLX02 200–540, 960–1,450 m	
	KLX04 100–992 m	
RSMBA	KLX02 540–960 m	Based on subdomain RSMBA03
RSMD	KLX02 1,450–1,700 m	Based on subdomain RSMD01
	KLX03 800–1,000 m	
RSMM	KLX03 100–620 m (A)	Based on subdomain RSMM01
	KLX03 620–800 m (D)	

In this report the characterisation of rock domains by borehole intervals has been modified so as to better represent the variability in thermal properties present within domains RSMA and RSMD (Table 5-3). Defined as a mixed zone with a large fraction of diorite/gabbro (501033), the RSMM domain occurs in south Laxemar. In borehole KLX03, it occurs between 100 and 800 m where it can be subdivided into a section dominated by Ävrö granite and a section dominated by quartz monzodiorite. Having only a minor component of rock type diorite/gabbro (501033), KLX03 is not considered representative for domain RSMM. It was therefore deemed more appropriate for thermal modelling purposes to allocate the two RSMM domain intervals in KLX03 to domain RSMA (dominated by Ävrö granite) and domain RSMD (dominated by quartz monzodiorite) respectively. For this reason modelling of domain RSMM has had to rely on estimates of typical rock type composition derived primarily from surface geological mapping /Wahlgren et al. 2005a/. For domain RSME borehole data is not available, so even in this case a rough estimate /Wahlgren et al. 2005a/ of rock type composition forms the basis for the thermal modelling.

Rock type distributions of the five lithological rock domains are illustrated in Table 5-4 and Table 5-5 where the dominant rock types are marked in red. When performing thermal modelling of the lithological domains for which borehole data is available, the rock type compositions for each domain is calculated (see Table 5-4 and Table 5-5). These differ slightly from the compositions presented in the geological model /SKB 2006/. There are two major reasons for this. Firstly, there is a difference in the basic data since fewer boreholes have been used in the thermal domain modelling than in the geological model. In the geological model borehole data from Simpevarp subarea is included, whereas for the thermal model presented here data is derived from Laxemar only. Secondly, as described above, the assignment of borehole intervals to domains deviates somewhat from that adopted in the geological model. For rock type compositions of the borehole intervals constituting each lithological domain (also calculated in the thermal domain modelling), see Section 5.4.1.

For convenience the domains are frequently referred to in their abbreviated form, e.g. A for domain RSMA.

Table 5-3. Data used for characterisation of rock domains for modelling of thermal properties.

Domain	Source of data for modelling
RSMA	KLX01 0–701 m
	KLX02 200–540, 960–1,000 m
	KLX04 100–990 m
	KLX03 100–620 m
RSMBA	KLX02 540–960 m
RSMD	KLX03 620–1,000 m
RSMM	Estimates of typical rock type compositions from geological mapping /Wahlgren et al. 2005a/.
RSME	Estimates of typical rock type compositions from geological mapping /Wahlgren et al. 2005a/.

Table 5-4. Comparison between rock type percentages (%) used in the thermal domain modelling and in the geological model for domains RSMA, RSMBA and RSMD. Dominant rock types are marked in red.

	Domain RSMA (Ävrö granite)		Domain RSMBA (Mixture of Ävrö granite and Fine-grained dioritoid)		Domain RSMD (Quartz monzodiorite)	
Rock name	**Modelling**	**Geological model**	**Modelling**	**Geological model**	**Modelling**	**Geological model**
Ävrö granite	82.27	54–92	57.93	57	2.50	present[1]
Fine-grained dioritoid	1.18	2–21	32.17	32	0.68	present[1]
Quartz monzodiorite	4.34	1–14			84.39	95
Pegmatite	0.24	0–1	0.12	1	1.11	0.3
Diorite/gabbro	3.02	0–12				
Fine-grained diorite-gabbro	4.07	0–5	7.86	8	7.18	present[1]
Granite	1.47			1	0.55	
Fine-grained granite	3.39	1–22	1.93	1	3.58	4

[1] No quantitative estimate available.

Table 5-5. Comparison between rock type percentages (%) used in the thermal domain modelling and in the geological model for domains RSME and RSMM. Dominant rock types are marked in red.

	Domain RSME (diorite/gabbro)		Domain RSMM (Mixed zone with large fraction of diorite/gabbro)	
Rock name	**Modelling[2]**	**Geological model**	**Modelling[2]**	**Geological model**
Ävrö granite			53	38–73
Fine-grained dioritoid			2	1–3
Quartz monzodiorite			27	0–27
Pegmatite			0	0–0.3
Diorite/gabbro	95	not quantified	12	1–36
Fine-grained diorite-gabbro			0	0–3
Granite			5	0–26
Fine-grained granite	5	not quantified	1	1–16

[2]Based on surface geological mapping /Wahlgren et al. 2005a/.

5.1.2 Borehole data

In boreholes where Ävrö granite is present, both accurate density loggings and a lithological classification of the borehole are required in order to model thermal conductivity. In boreholes without Ävrö granite only a rock classification of the borehole is required. The rock type classifications need to be current with both dominant and subordinate rock types described using 6-digit codes.

The status of available input data regarding rock type classifications (lithology) and density loggings is as follows:

- KLX01, KLX02, KLX03, KLX04, KAV04A: Calibrated and filtered density loggings available for all five boreholes. Density logging for KLX01 were carried out by Malå Geoscience in the 1980's and are considered to be less accurate than more recent loggings.
- KLX01, KLX02, KLX03, KLX04, KAV04A: Rock type classifications are available for all boreholes. In the case of KLX02, subordinate rock types may be described either by four-digit or six-digit descriptions. Where only four digit descriptions are available for subordinate rock types, upgrading was performed by adding 50 in front of the four-digit code. Subordinate rock types in KLX01 were logged by Petrocore (1995 and 1998) using four-digit codes. These were also adjusted to corresponding six-digit descriptions.

5.2 Conceptual model of spatial variability

There are three main causes for the spatial variability of thermal conductivity at the domain level; (1) small scale variability between minerals, (2) spatial variability within each rock type, and (3) variability between the different rock types making up the domain. The first type entails variability in small samples (based on TPS measurements and modal analysis). At this scale, the small scale variability can be substantial. However, the variability is rapidly reduced when the scale increases.

The second type of variability is associated with variability in sample data from a rock type and cannot be explained by mineral scale variations. This is believed to be especially important for the rock type Ävrö granite. Variograms of thermal conductivity for different boreholes indicate variability at different scales. Although there are differences from one borehole to another, at least 30% of the variability within Ävrö granite occurs at scales of less than about 2 m. This subject is treated in more detail in 4.7.2.

The third type of variability is due to the presence of different rock types in the lithological domain. This variability is more pronounced where the difference in thermal conductivity is large between the most common rock types of the domain. Large variability of this type can also be expected in a domain of many different rock types. It is believed that the variability between rock types is important for all defined domains. It is only reduced significantly when the scale becomes large compared to that of the spatial occurrence of the rock type.

Of importance at the domain level is the scale relevant for the canister, i.e. at which the thermal conductivity is important for the heat transfer from the canister. At present knowledge /Sundberg et al. 2005a/, variability below 1 m seems to have little or no relevance for the canister temperature. Therefore, the approach in the domain modelling is to use results mainly from 0.8 m scale so as not to underestimate the scale effect, and to draw conclusions of representative thermal conductivity values from that.

5.3 Modelling approach for domain properties

5.3.1 Introduction

The methodology for thermal conductivity domain modelling and the modelling of scale dependency were developed for the Prototype Repository at the Äspö HRL /Sundberg et al. 2005a/. The methodology involves a base approach, main approach in /Sundberg et al. 2005a/, by which the mean thermal conductivity at domain level is modelled (see Figure 5-3), and a number of complementary approaches which are applied in order to evaluate the spatial variability at domain level. The base approach is applied to the lithological domains RSMA (Ävrö granite), RSMBA (Mixture of Ävrö granite and fine-grained dioritoid), and RSMD (quartz monzodiorite). The approach differs slightly depending on whether borehole density loggings can or cannot be used. Rock domains RSMM and RSME are not represented by any boreholes and therefore Monte Carlo simulation is used as the base approach. For these domains, the base approach does not involve any upscaling.

When evaluating the spatial variability at domain level using the four alternative/complementary approaches (Approach 1–4) /Sundberg et al. 2005a/, it is assumed that spatial variability for a domain can be estimated as the sum of the variance due to different rock types and the variance due to spatial variability within the dominant rock types:

$$V_{tot} = V_{between\ rock\ type} + V_{within\ rock\ type} \qquad \textit{Equation 5-1}$$

The "between rock type" variability is qualitatively different from, and therefore likely to be independent of, the "within rock type" variability. Therefore, adding the two types of variances is considered reasonable.

Table 5-6 summarises the different approaches applied to the respective domains. These approaches and the results are described in more detail below.

Table 5-6. Modelling approaches used for different domains. For domains RSME and RSMM no representative borehole data are available.

Domain	Modelling approach					
	Base approach		Approach 1	Approach 2	Approach 3	Approach 4
	Modelling from borehole data	Monte Carlo simulation				
RSMA	X			X	X	X
RSMBA	X			X	X	X
RSMD	X		X		X	X
RSMM		X				
RSME		X				

5.3.2 Base approach

The main purpose of the base approach is to determine the mean thermal conductivity of each domain. The base approach using borehole data was applied to domains RSMA, RSMBA and RSMD. This approach is described in detail in /Sundberg et al. 2005a/ and is summarised below.

Each borehole belonging to a domain is divided into 0.1 m long sections and each section is assigned a thermal conductivity value according to the lithological classification of that section. Both dominant and subordinate rock types are considered in this context. The principle for assignment of thermal properties is illustrated in Figure 5-1.

The next step is the upscaling from the 0.1 m scale to an appropriate scale. The upscaling is performed on a range of scales, from 0.1 m up to approximately 60 m. The upscaling is performed in the following way, illustrated both in Figure 5-1 and Figure 5-2:

1. The boreholes representing the domain are divided into a number of sections with a length according to the desired scale.

2. Thermal conductivity is calculated for each section as the geometric mean of the values at the 0.1 m scale. This gives the effective thermal conductivity at the desired scale.

3. The mean and the variance of all sections at the desired scale are calculated. For each scale, the calculations are repeated *n* times with different assignment of thermal conductivity values at the 0.1 m scale (stochastic simulation). This produces representative values of the mean and the standard deviation for the desired scale.

In Figure 5-1, 25 sections are indicated, each with a length of 0.1 m. For the scale 0.5 m, the thermal conductivity $\lambda_{0.5-1}$ is estimated as the geometric mean of five 0.1 m sections, $\lambda_{0.5-2}$ as the geometric mean for the next five 0.1 m sections, and so on. The mean and variance is then easily computed for the 0.5 m scale. This sequence is repeated for the other scales of interest. The effect of upscaling is illustrated in Figure 5-2.

As illustrated in Figure 5-3, the base approach is slightly different between domains where density loggings can be used (domains RSMA and RSMBA, dominated by Ävrö granite) or cannot be used (domain RSMD). The reason is that density loggings of Ävrö granite can be used for domain RSMA and RSMBA to take into account spatial correlation within the dominant rock type. This is not possible for domain RSMD (quartz monzodiorite), which is dominated by other rock types for which no reliable "within rock type" relationship is presently available. Therefore, the variance for domain RSMD is underestimated in the base approach. This is the main disadvantage of the base modelling approach. The spatial variability within the dominant rock type needs to be added, see alternative approaches below.

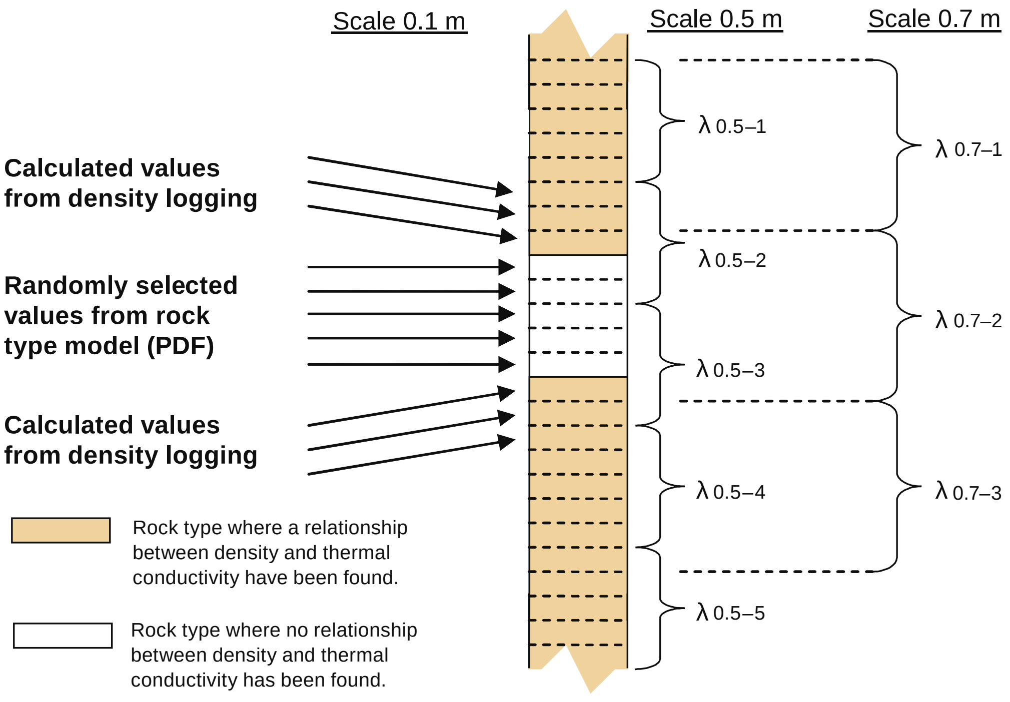

Figure 5-1. *Thermal conductivity is assigned to 0.1 m sections by calculation from density loggings or randomly selected from the rock type models. Upscaling is performed by calculating geometric means for different scales, for example 0.5 and 0.7 m.*

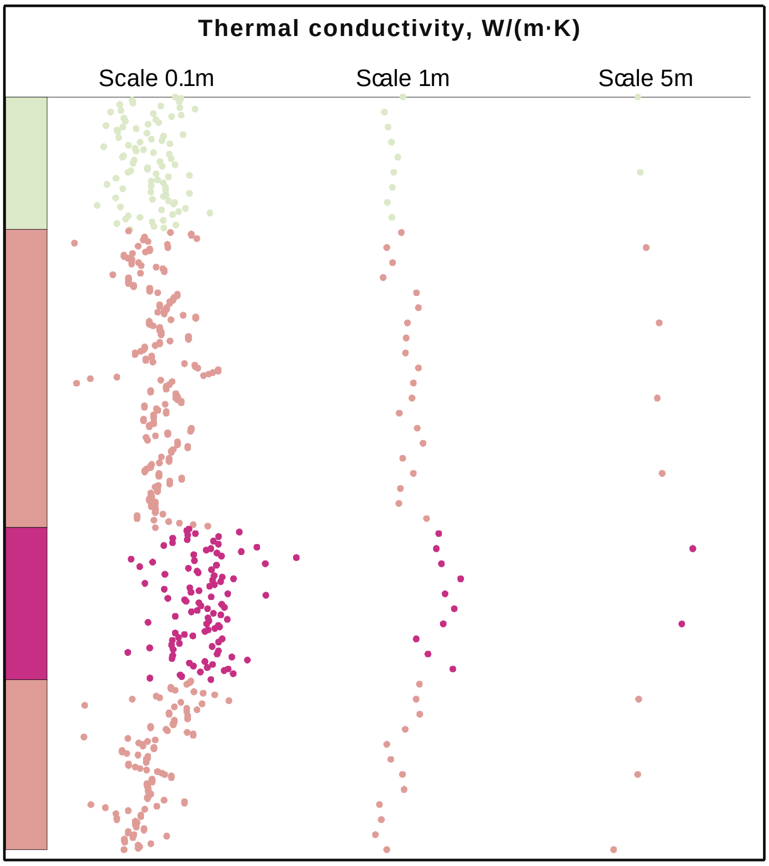

Figure 5-2. *Effects of applying the principle for upscaling of thermal conductivity, as given in Figure 5-1. As can be seen, the spatial variability within the rock types is levelled out due to the modelling concept.*

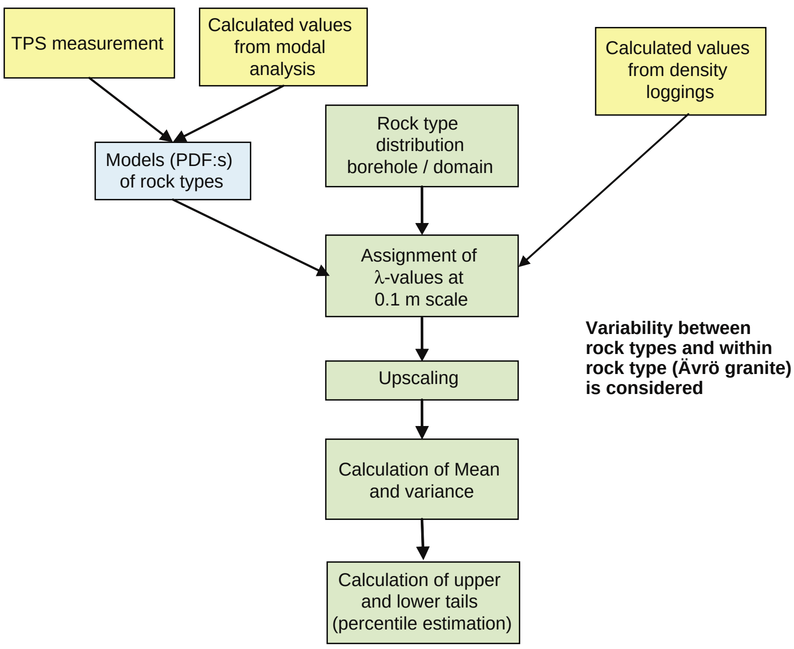

Figure 5-3. *Base approach for estimation of thermal conductivity for domains RSMA (Ävrö granite) and domain RSMBA (Mixture of Ävrö granite and fine-grained dioritoid) and RSMD. Yellow indicates the data level, blue the rock type level, and green the domain level. The parameter λ refers to thermal conductivity.*

Even for domains RSMA and RSMBA there is a possibility of the “within rock type” variance being underestimated since only 82% and 55% respectively of the boreholes comprising these domains consists of Ävrö granite. The variance due to the remaining rock types is not accounted for. However, the “within rock type” variability is almost certainly of greater importance for Ävrö granite than for the other rock types.

Upper and lower tails of the distributions can be derived directly from the results of the stochastic simulation. No assumption of the type of statistical distribution of the thermal conductivity values is required. In this study spatial variability within rock types is estimated for the 0.8 m scale only. In order not to underestimate the variance due to different uncertainties, it is assumed that the thermal conductivity which is representative of the domain in canister scale is equal to the thermal conductivity in the 0.8 m scale.

Another type of base approach is applied to rock domains RSME (diorite/gabbro) and RSMM (Mixed zone with large fraction of diorite/gabbro), which are not represented by any boreholes and must therefore be treated differently. For these domains a simplified approach based on Monte Carlo simulation has been used. The PDF models for the rock types present in these domains (Table 4-22) are used to estimate the variability at the 0.1 m scale. No direct upscaling is possible due to lack of borehole data.

Although domain M comprises a large percentage of Ävrö granite it is has not been modelled using density loggings. Thus, spatial variability within the rock types comprising this domain has not been taken into account.

Theory of upscaling[1]

The geometrical mean equation, referred to above, is used to produce an effective thermal conductivity in an appropriate scale from small scale determinations. The geometric mean equation is associated with transport in 2D and is often applied for estimation of effective transport properties /Dagan 1979, Sundberg 1988/. However, the effective transport properties are influenced by the variance, which is not considered when the geometric mean is calculated. According to /Gutjahr et al. 1978/ and /Dagan 1979/, the effective hydraulic conductivity is slightly different due to the dimensionality of the problem. /Dagan 1979/ derived the following general solution to the effective mean hydraulic conductivity (transformed to thermal conductivity):

$$\lambda_e = +(m-1)\cdot\lambda_x+(\int f(\lambda)\, d\lambda / (m+1)\cdot\lambda_x+\lambda)^{-1} \qquad \textit{(Equation 5-2)}$$

Where m is the dimensionality of the problem and f(λ) the frequency function. If λ_x is substituted with λ_{max} and λ_{min}, the result is Hashin’s and Shtrikman’s well known upper and lower bounds for an isotropic material /Hashin and Shtrikman 1962/. If λ_x is substituted with λ_e, the self consistent approximation (SCA) is obtained as follows:

$$\lambda_e = 1/m\cdot(\int f(\lambda)\, d\lambda / (m+1)\cdot\lambda_e+\lambda)^{-1} \qquad \textit{(Equation 5-3)}$$

For a lognormal distribution, the effective conductivity according to Equation 5-3 for two dimensions (*m* = 2) coincides with the geometric mean. For three dimensions (*m* = 3) the effective conductivity is slightly higher. Equation 5-3 is used to calculate the thermal conductivity from the mineral distribution of rocks /Sundberg 1988/.

If the standard deviation (σ) of the $\log_{10}$ (λ) is small, the effective thermal conductivity can be approximated as follows for a lognormal conductivity distribution:

---

[1] The text on the theory of upscaling is essentially an extract from /Sundberg et al. 2005a/.

2D: $\lambda_e = \lambda_G$ *(Equation 5-4)*

3D: $\lambda_e = \lambda_G [1+\sigma^2/6]$ *(Equation 5-5)*

where λ_G is the geometric mean thermal conductivity. However, in this thermal application the variance is low and therefore the geometric mean is an adequate approximation /Sundberg et al. 2005a/.

5.3.3 Approach 1: Addition of within rock variability from domain RSMA

The following method to estimate the spatial variability within the dominant rock types for which density loggings are unavailable was employed in the thermal modelling work for the Simpevarp subarea /Sundberg et al. 2005b/, and is replicated here. Variance caused by spatial variability within Ävrö granite was estimated for domain RSMA. This was achieved by performing two simulations, one (A) in which the thermal conductivities are calculated both from PDF models and density loggings, resulting in both "between rock type" and "within rock type" variability, the other (C) whereby all thermal conductivity values are randomly selected from the rock type PDF models and no data from density loggings are used, resulting in only "between rock type" variability. The variance contributed by spatial correlation within rock types is assumed to be the difference between simulation (A) and (C), see Figure 5-4.

It was assumed that the variance caused by spatial variability within other dominant rock types is identical to spatial variability within rock type Ävrö granite in domain RSMA. The "within rock type" variance for Ävrö granite in domain RSMA is then added to the "between rock type" variance calculated for other domains. This is likely to result in an overestimation of the spatial variability, since heterogeneity within Ävrö granite is expected to be larger than for other rock types. The addition of variances, according to Equation 5.1 is assumed to be valid. This approach has been applied to domain RSMD, which is dominated by quartz monzodiorite.

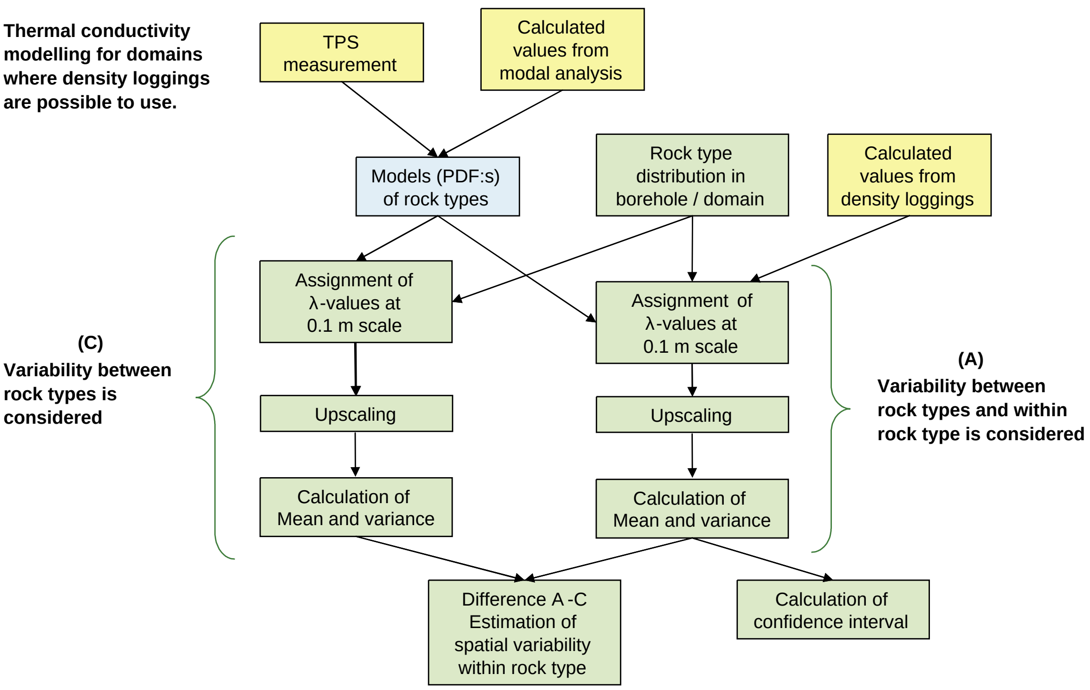

Figure 5-4. *Approach for estimation of "within rock type" spatial variability for domains where density loggings are applicable, namely RSMA (Ävrö granite) and domain RSMBA (Mixture of Ävrö granite and fine-grained dioritoid). Yellow colour indicates the data level, blue the rock type level, and green the domain level. The parameter λ refers to thermal conductivity.*

5.3.4 Approach 2: Extrapolation of spatial variability

When modelling domains RSMA (dominated by rock type Ävrö granite) and RSMBA (mix of Ävrö granite and fine-grained dioritoid) according to the base approach, spatial distribution was only considered for 81.5% and 55.5% respectively of the borehole lengths, since not all 0.1 m sections of the domain were comprised of Ävrö granite, the only lithology for which density logging data could be used. In addition, some density logging data for Ävrö granite may be outside the range for which the model relationship is considered valid, see 4.5.2. For the remainder of the borehole length, 18.5% and 44.5% respectively, thermal conductivity values were randomly assigned from the rock type models. Therefore, an approach was applied to correct for this. It is assumed that all rock types have the same spatial variation as Ävrö granite. By randomly replacing thermal conductivity values estimated from density logging with random PDF values it is possible to study the effect of ignoring the "within rock type" spatial variability for parts of the borehole. By repeating this exercise for successively larger parts of the borehole, it is possible to construct a graph of how the variance is affected. This curve can be extrapolated to 100% in order to determine the total "within rock type" variance. In this approach it is implicitly assumed that the spatial variation of other rock types is similar to that of Ävrö granite. It is reasonable to assume that the total variance is overestimated with this approach because the heterogeneity of Ävrö granite is expected to be larger than for other rock types.

5.3.5 Approach 3: Subtraction of small scale variability

In the third approach, variograms are used to estimate the small scale variance of Ävrö granite in RSMA. The variograms are based on density logging data from boreholes KLX01, KLX02, KLX03 and KLX04, all of which have sections belonging to domain RSMA. In this approach, the small-scale variability for the scale of interest (0.8 m) within Ävrö granite is subtracted from the total variability of the same rock type (from PDF:s). This residual variability is assumed to be the variance after upscaling. The basis for the approach is that variability at scales smaller than the desired is evened out. A limitation of this approach is that data to construct variograms are available for Ävrö granite only. For domain RSMD it was assumed that the small scale variability within quartz monzodiorite is of the same relative magnitude as for Ävrö granite. This assumption is considered reasonable since both Ävrö granite and quartz monzodiorite are granitoid rocks with similar grain size.

Variograms presented in Figure 5-5 are used to estimate the small-scale variance of Ävrö granite, the dominant rock type in domain RSMA.

The variograms of the various boreholes (Figure 4-36 to Figure 4-39), however, illustrate that there is a difference between the boreholes regarding spatial correlation. As pointed out in the Simpevarp thermal modelling work /Sundberg et al. 2005b/, where data from only two boreholes were available, the results may not be entirely representative. Four boreholes are used to represent domain RSMA in the Laxemar subarea, which should lead to an improvement in this regard.

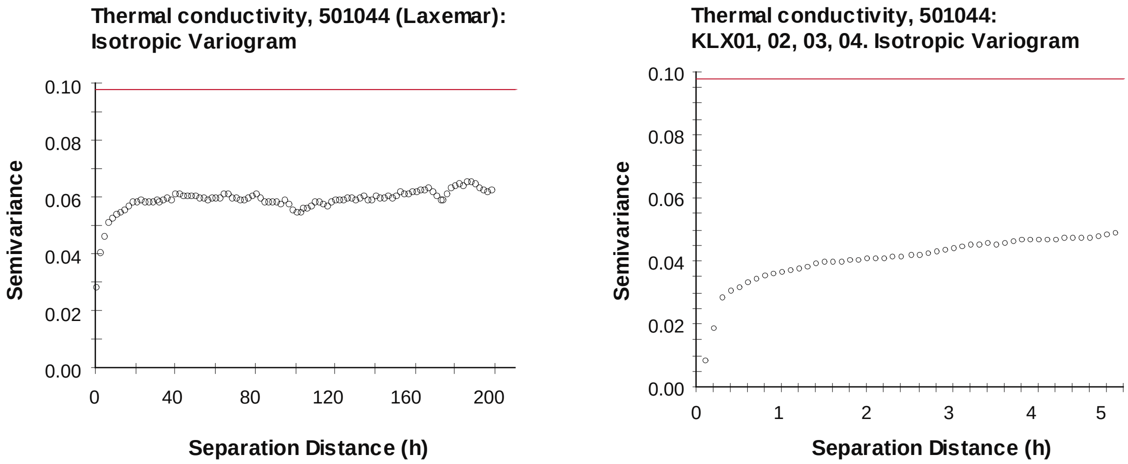

Figure 5-5. *Variogram of thermal conductivity for Ävrö granite (501044)in domain RSMA in boreholes KLX01, KLX02, KLX03 and KLX04, estimated from density logging; 0–200 m and 0–5 m separation distance. The straight line indicates the total variance in the data. Separation distance is expreesed in metres, whereas the unit of semivaruiance is (W/(m·K))²*.

5.3.6 Approach 4: Upscaling of "within rock type" variability

In this approach /Sundberg et al. 2005a/, the spatial variability within the dominant rock type is estimated based on TPS measurements or density loggings. Analysis of TPS data can provide a rough estimation of the spatial variability within the rock type. TPS measurements are classified in spatial groups depending on their location and the geometric mean is calculated for each group. This gives a set of data for the scale in question (based on the spatial groups). The variance for this data set is a rough estimate of the variance for the desired scale. This procedure can be repeated for different scales and the resulting variances can be plotted against the scale on a graph (see Figure 5-29). The variance for the desired scale can be estimated from the graph and this "within rock type" variance is then added to the "between rock type" variance calculated in the base approach.

For domains with more than one dominant rock type, the variance V_2 is estimated as the weighted sum of the spatial variance for the different dominant rock types, where the weighting factors are the fractions of the respective rock types in the domain. Although this approach only provides a rough estimate of the total variability it encompasses all the major types of variability within the domain.

5.4 Domain modelling results

5.4.1 Borehole modelling

Figure 5-6 to Figure 5-10 shows the modelled thermal conductivity plotted against lithological logs and borehole length for boreholes KLX01, KLX02, KLX03, KLX04 and KAV04A. These results are summarised in Table 5-7 for the 0.8 scale. Borehole KAV04A is located in Simpevarp subarea and is not included in the modelling of Laxemar. It is used instead to complement the results of the Simpevarp model version 1.2.

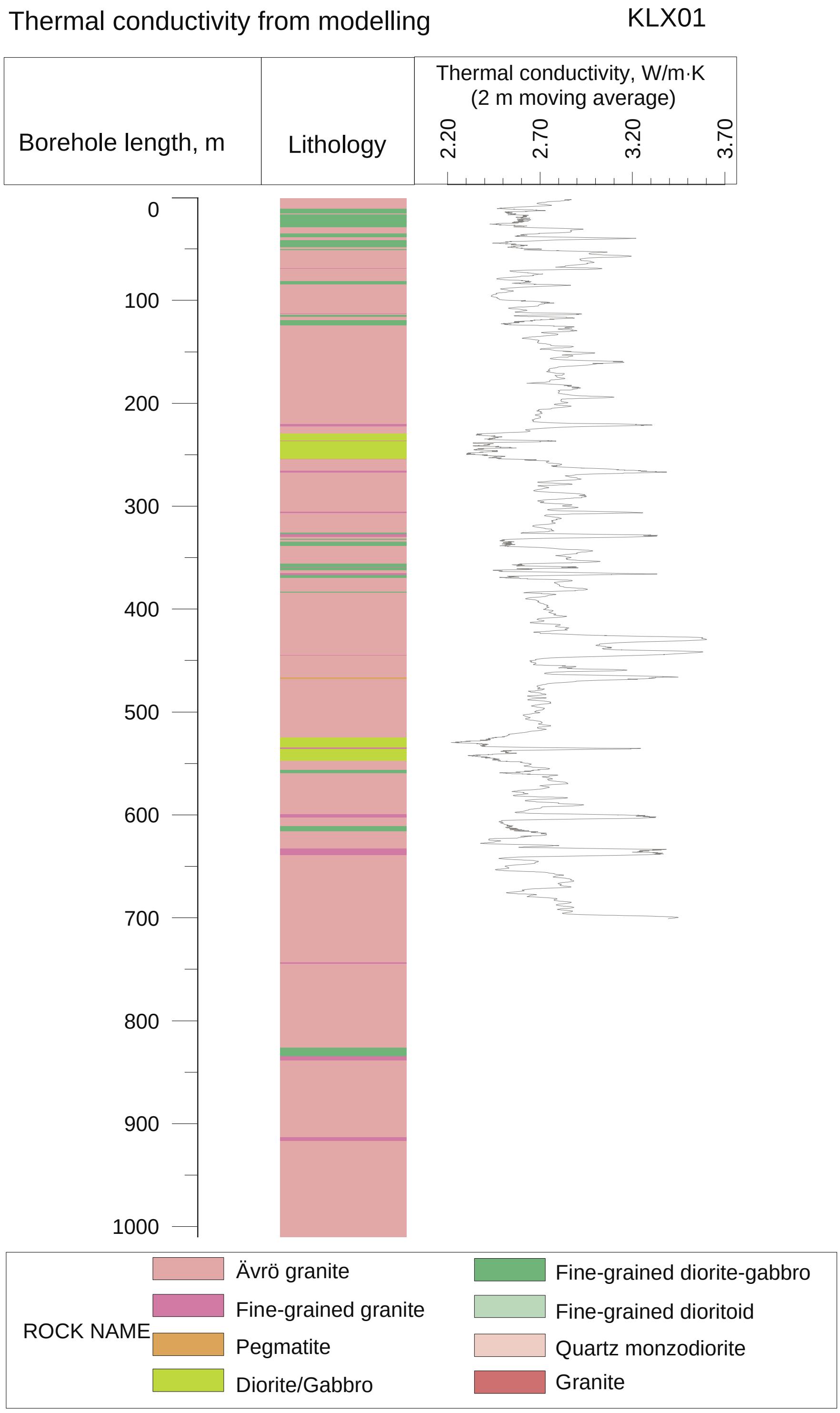

Figure 5-6. *Exemplification of changes in thermal conductivity along borehole KLX01. Thermal conductivity is calculated as geometrical means over 2 m long sections (moving average) from 0.1 m data. The results originate from one realisation only, and are based on both deterministic (for Ävrö granite) and stochastic (for other rock types) computations.*

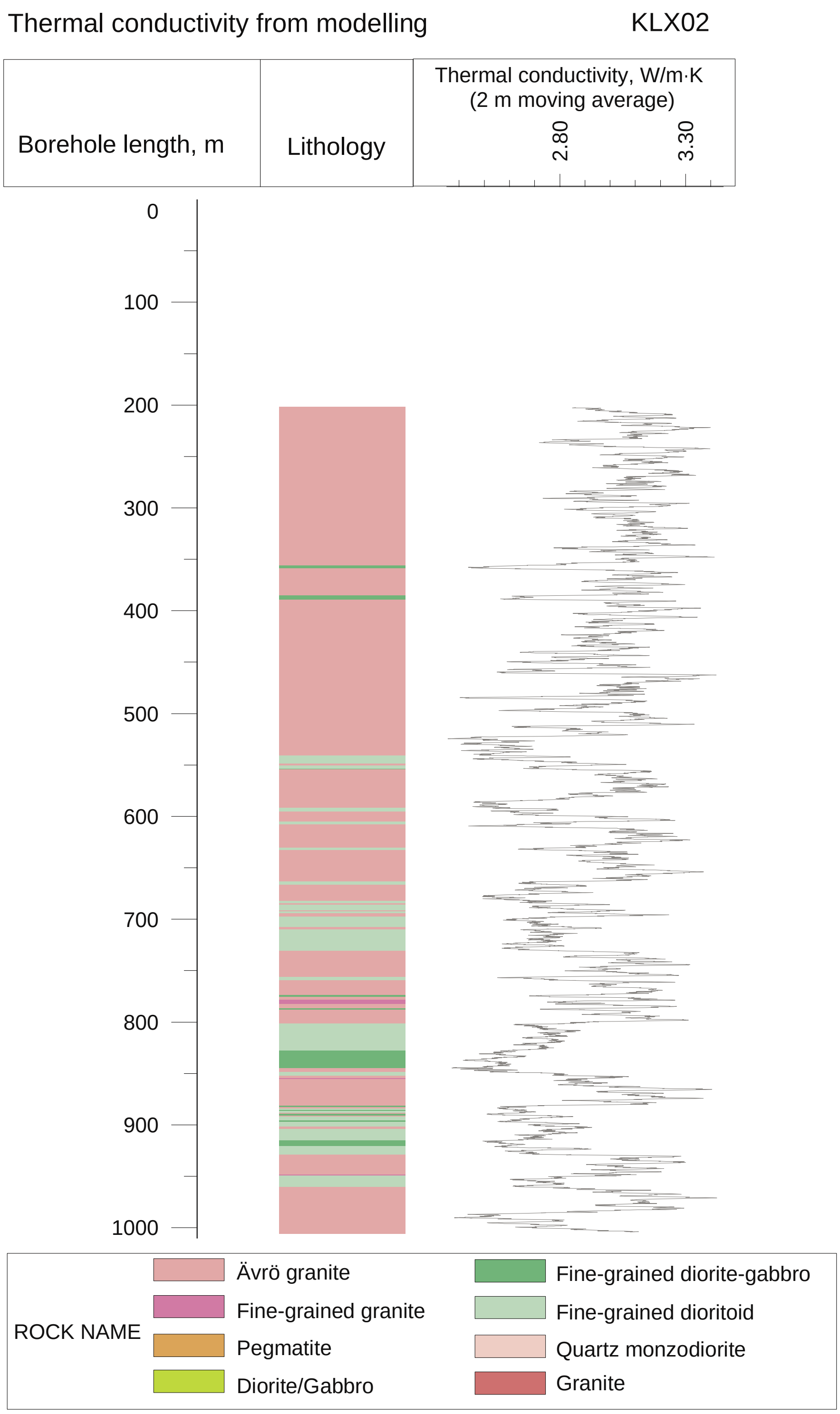

Figure 5-7. *Exemplification of changes in thermal conductivity along borehole KLX02. Thermal conductivity is calculated as geometrical means over 2 m long sections (moving average) from 0.1 m data. The results originate from one realisation only, and are based on both deterministic (for Ävrö granite) and stochastic (for other rock types) computations.*

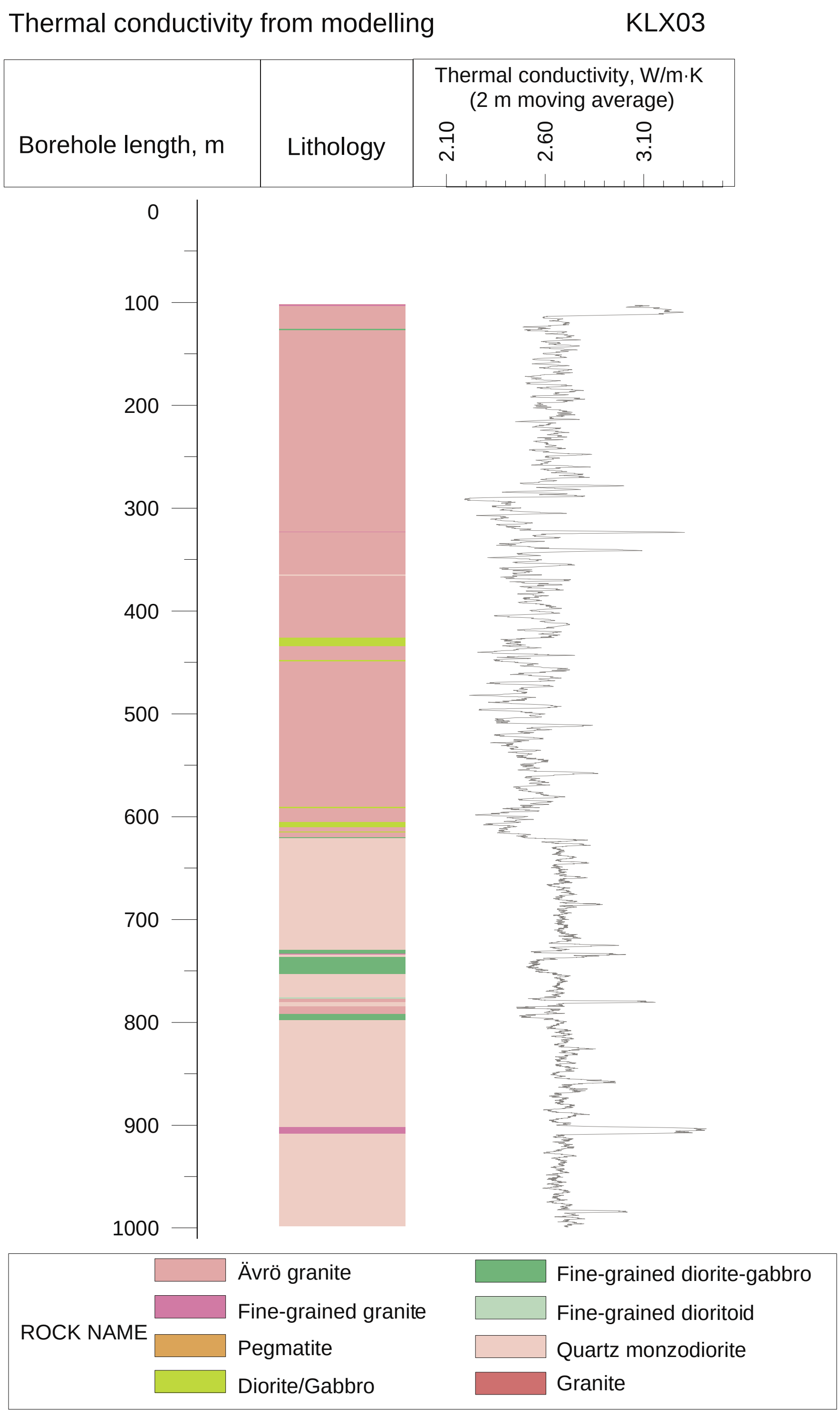

Figure 5-8. *Exemplification of changes in thermal conductivity along borehole KLX03. Thermal conductivity is calculated as geometrical means over 2 m long sections (moving average) from 0.1 m data. The results originate from one realisation only, and are based on both deterministic (for Ävrö granite) and stochastic (for other rock types) computations.*

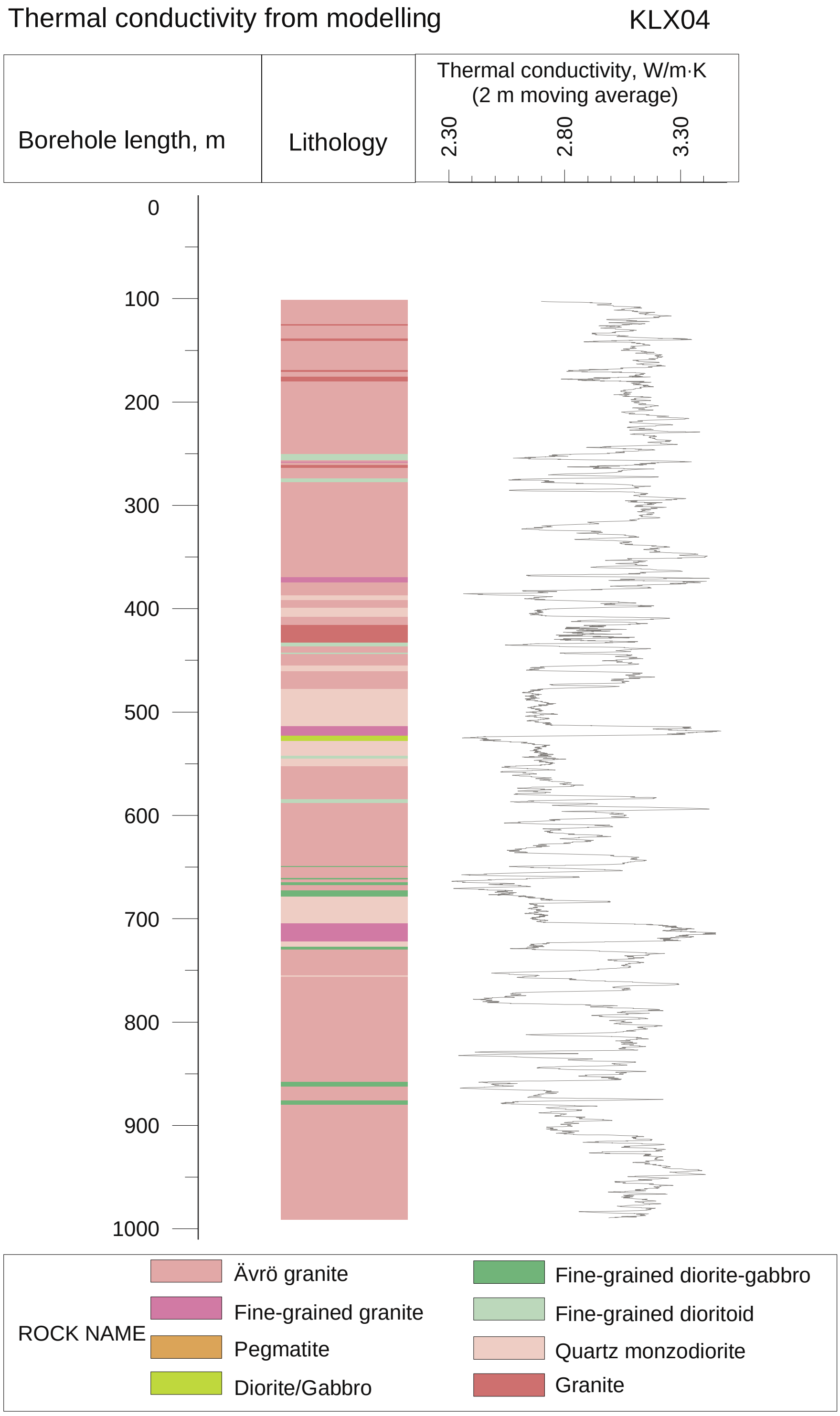

Figure 5-9. *Exemplification of changes in thermal conductivity along borehole KLX04. Thermal conductivity is calculated as geometrical means over 2 m long sections (moving average) from 0.1 m data. The results originate from one realisation only, and are based on both deterministic (for Ävrö granite) and stochastic (for other rock types) computations.*

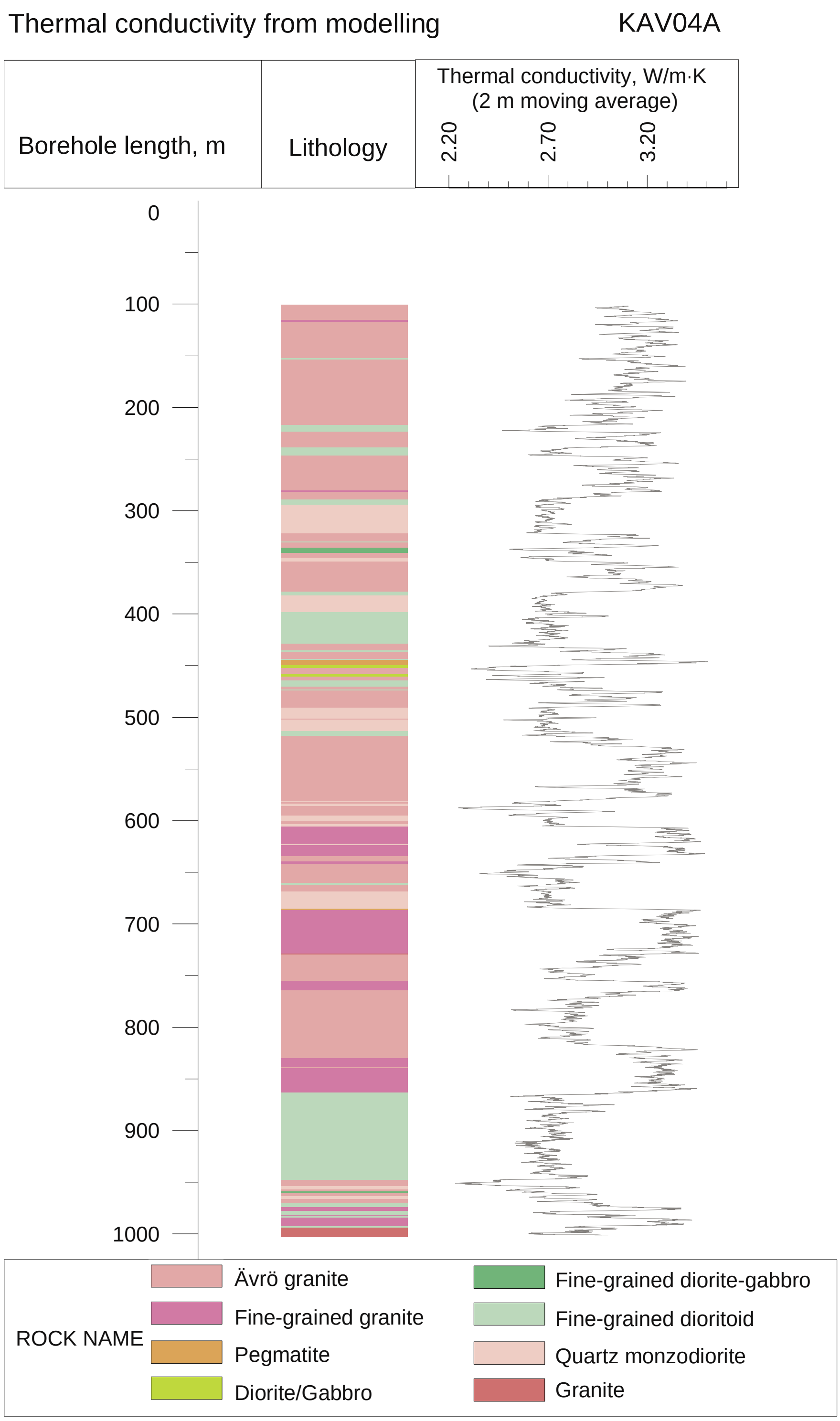

Figure 5-10. *Exemplification of changes in thermal conductivity along borehole KAV04A. Thermal conductivity is calculated as geometrical means over 2 m long sections (moving average) from 0.1 m data. The results originate from one realisation only, and are based on both deterministic (for Ävrö granite) and stochastic (for other rock types) computations. Not included in Laxemar 1.2 model.*

Table 5-7. Summary of thermal conductivity (W/(m·K)) modelling results at 0.8 m scale for boreholes KAV04A, KLX01, KLX02, KLX03 and KLX04.

Borehole	Scale, m	Mean	Std dev	Comment
KAV04A	0.8	2.951	0.284	Not included in Laxemar 1.2 model. Used to complement Simpevarp 1.2 model.
KLX01	0.8	2.751	0.233	
KLX02	0.8	2.927	0.258	
KLX03	0.8	2.627	0.171	
KLX04	0.8	2.946	0.254	

5.4.2 Domain modelling: base approach

Domain RSMA, Ävrö granite

Domain RSMA is dominated by the rock type Ävrö granite (501044) which constitutes approximately 80% of the domain. The modelling of domain RSMA is based on data from four boreholes: KLX01, KLX02, KLX03 and KLX04. Approximately 98% of the thermal conductivity values for Ävrö granite are computed from density loggings. For the rock type distribution of the domain and of the boreholes which constitute the domain, see Table 5-8.

Modelling results for domain A at the 0.8 m scale are presented in Table 5-8 and Figure 5-11. The lowest modelled thermal conductivity at this scale is 2.09 W/(m·K), which is somewhat lower than the lowest value measured in the laboratory for Ävrö granite (2.16 W/(m·K)). A majority of the extremely low values are derived from density loggings

Table 5-8. Modelling results for domain RSMA (Laxemar subarea) and its comprising borehole sections: mean and standard deviation of thermal conductivity (W/(m·K)) for 0.8 m scale and rock type distributions in percent.

	Domain RSMA	KLX01	KLX02	KLX03	KLX04
		Borehole interval			
		1–701 m	201.5–540 m 960–1,000 m	100–620 m	100–990 m
Rock name	**Percentages of rock types**				
Ävrö granite (501044)	82.3	80.0	96.4	92.1	72.2
Fine-grained dioritoid (501030)	1.2	0	0	0.4	3.1
Quartz monzodiorite (501036)	4.3	0	0	0.5	11.9
Pegmatite (501061)	0.2	0.4	0.2	0.1	0.3
Diorite/gabbro (501033)	3.0	6.4	0	4.9	0.6
Fine-grained diorite-gabbro (505102)	4.1	9.1	2.5	0.6	2.8
Granite (501058)	1.5	0	0	0.1	4.0
Fine-grained granite (511058)	3.4	4.1	1.0	1.3	5.0
	Thermal conductivity				
Mean (0.8 m scale)	2.82	2.75	3.0	2.57	2.95
Std dev	0.281	0.23	0.25	0.18	0.26
Mean (0.1 m scale)	2.83				
Std dev	0.337				
Mean (2 m scale)	2.82				
Std dev	0.261				

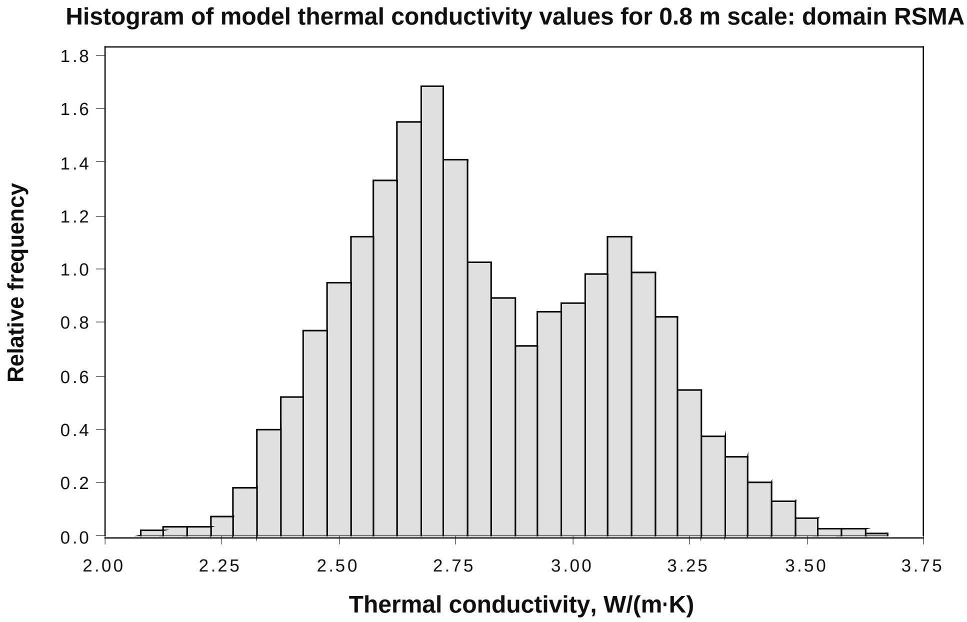

Figure 5-11. *Histogram of thermal conductivities for domain RSMA at the 0.8 m scale using the base approach.*

for Ävrö granite, and are not merely an effect of using probability density functions as rock type models. The results of modelling for the individual boreholes are also presented in Table 5-8. Of particular interest is the large difference in thermal conductivity between boreholes making up domain RSMA. KLX03 displays the lowest thermal conductivity values whereas KLX02 and KLX04 have the highest values. The bimodal distribution and large variance at domain level reflects the characteristic bimodal frequency distribution of the dominant rock type, i.e. Ävrö granite. Figure 5-11 clearly shows that assuming a normal distribution would be incorrect. This has implications for the estimation of percentiles, see 5.4.2.

The means and standard deviations of thermal conductivity calculated at different scales are displayed in Figure 5-12 and Figure 5-13. It is worth noting the changes in mean and, in particular, standard deviation that occur as a result of upscaling. As can be seen in Figure 5-12, the differences are greatest at scales below 2 m.

The results of domain modelling in Laxemar can be compared with those of Simpevarp subarea. In the site descriptive model for Simpevarp version 1.2, thermal conductivity was modelled for domain RSMA based on boreholes KAV01 and KLX02. Only the first of these is located in Simpevarp subarea, the other, KLX02, is used in this report to characterise the Laxemar subarea. The recently acquired data for KAV04A can, together with KAV01, be used to describe and model this domain within the Simpevarp subarea. The results according to the base approach are presented in Table 5-9. Compared to the Laxemar subarea a slightly higher mean thermal conductivity (2.94 W/(m·K)) was derived for the Simpevarp subarea. Possible reasons for a higher value for Simpevarp subarea include a greater proportion of fine-grained granite and a lower proportion of low thermal conductivity Ävrö granite in Simpevarp.

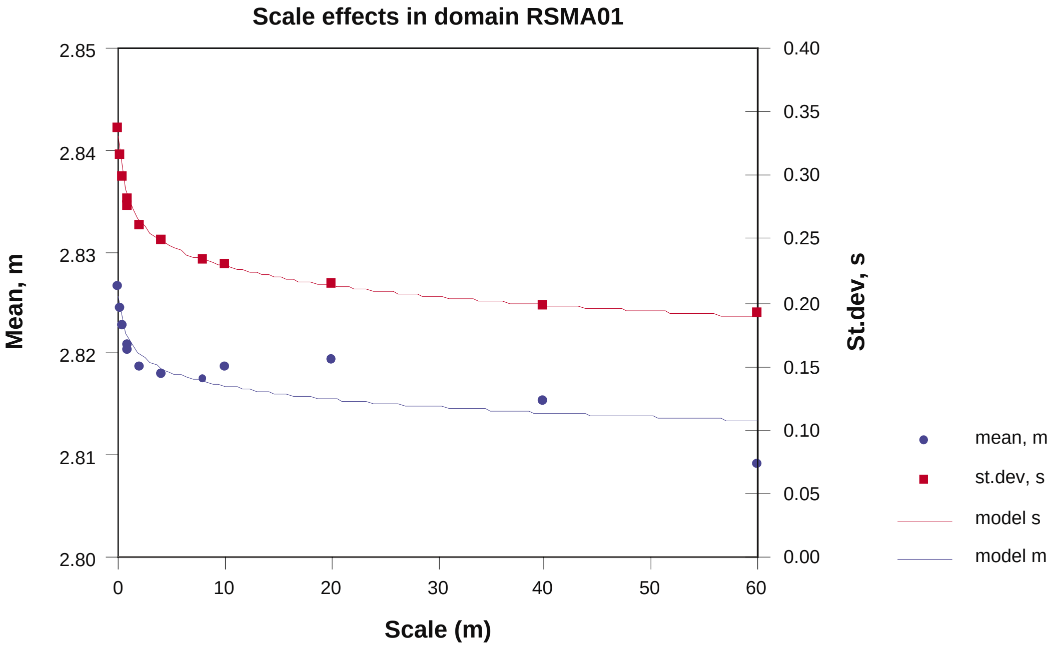

Figure 5-12. *Modelling results of thermal conductivity for domain RSMA: scale dependence (0.1 to 60 m) of mean and standard deviation. Logarithmic curves fitted to data.*

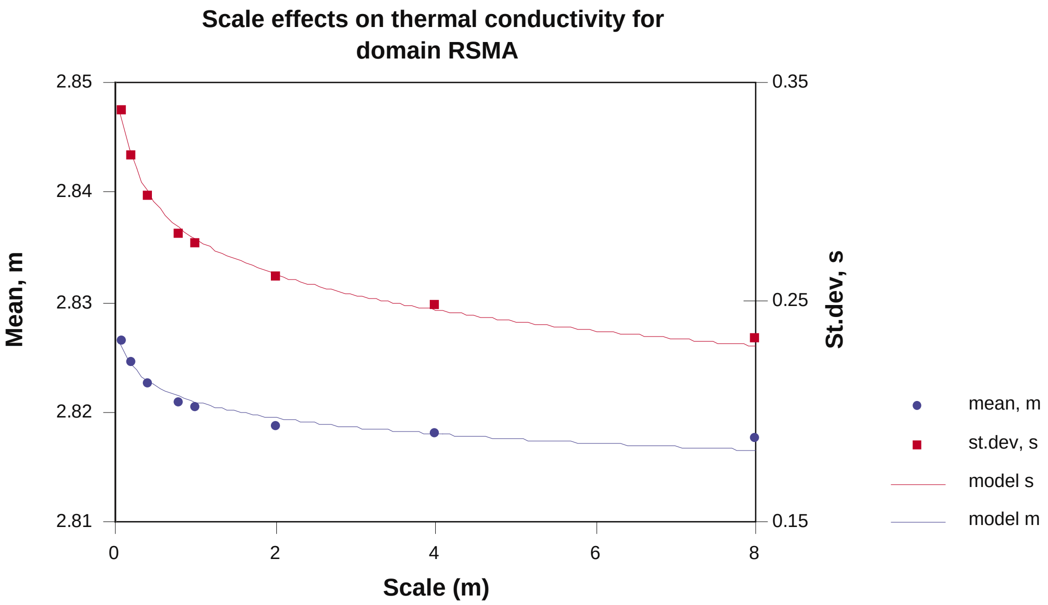

Figure 5-13. *Modelling results of thermal conductivity for domain RSMA: scale dependence (0.1 to 8 m) of mean and standard deviation. Logarithmic curves fitted to data.*

Table 5-9. Modelling results for domain RSMA (Simpevarp subarea) and its comprising borehole sections based on partly new data: mean and standard deviation of thermal conductivity (W/(m·K)) for 0.8 m scale and rock type abundances in percent.

	Domain RSMA	KAV01	KAV04
		Borehole interval	
		2.1–743 m	101.5–289 m 690–1,002 m
Rock name	**Percentages of rock types**		
Ävrö granite (501044)	70.8	82.0	54.0
Fine-grained dioritoid (501030)	13.7	8.6	21.4
Quartz monzodiorite (501036)	0.5	0	1.1
Pegmatite (501061)	0.5	0.5	0.5
Diorite/gabbro (501033)	0	0	0
Fine-grained diorite-gabbro (505102)	2.0	3.1	0.34
Granite (501058)	1.7	1.3	2.3
Fine-grained granite (511058)	10.9	4.5	20.3
	Thermal conductivity, W/(m·K), for 0.8 m scale		
Mean	2.94	2.89	3.0
Std dev	0.27	0.24	0.27

Figure 5-14 and Figure 5-15 illustrate the modelled (according to the base approach) thermal conductivity plotted against elevation for the different boreholes which constitutes domain RSMA (Ävrö granite). The plotted thermal conductivity values are calculated as geometrical mean values for 2 m and 50 m long sections (moving average) respectively. The influence of subordinate rock type sections is clearly visible as spikes in the figures, but the variability within rock types may be underestimated according to the base modelling approach.

Domain RSMBA, Mixture of Ävrö granite and fine-grained dioritoid

Dominant rock types in domain RSMBA are Ävrö granite (501044) and fine-grained dioritoid (501030), which constitute 58% and 32% of the domain respectively. Modelling of the domain is based on borehole section 540–960 m in KLX02 in subdomain RSMBA03, see Table 5-10. Subdomain RSMBA03 does not extend to the surface, i.e. it is found only at depth. Similar subdomains, RSMBA01 and RSMBA02, outcrop further south at the contact zone between Ävrö granite and quartz monzodiorite. Within rock variability is taken into account for Ävrö granite, for which density loggings can be employed. Thermal conductivities for other rock types are derived from the distributions models (PDF).

Modelling results for the domain at the 0.8 m scale is presented in Table 5-10 and Figure 5-16. Of particular interest here is the tendency towards bimodality for the data distribution. This reflects both the variability between dominant rock types (Ävrö granite and fine-grained dioritoid) and the within Ävrö granite variability. Increasing the scale from 0.1 m to 0.8 m reveals a trend towards a less normal and more skewed data distribution.

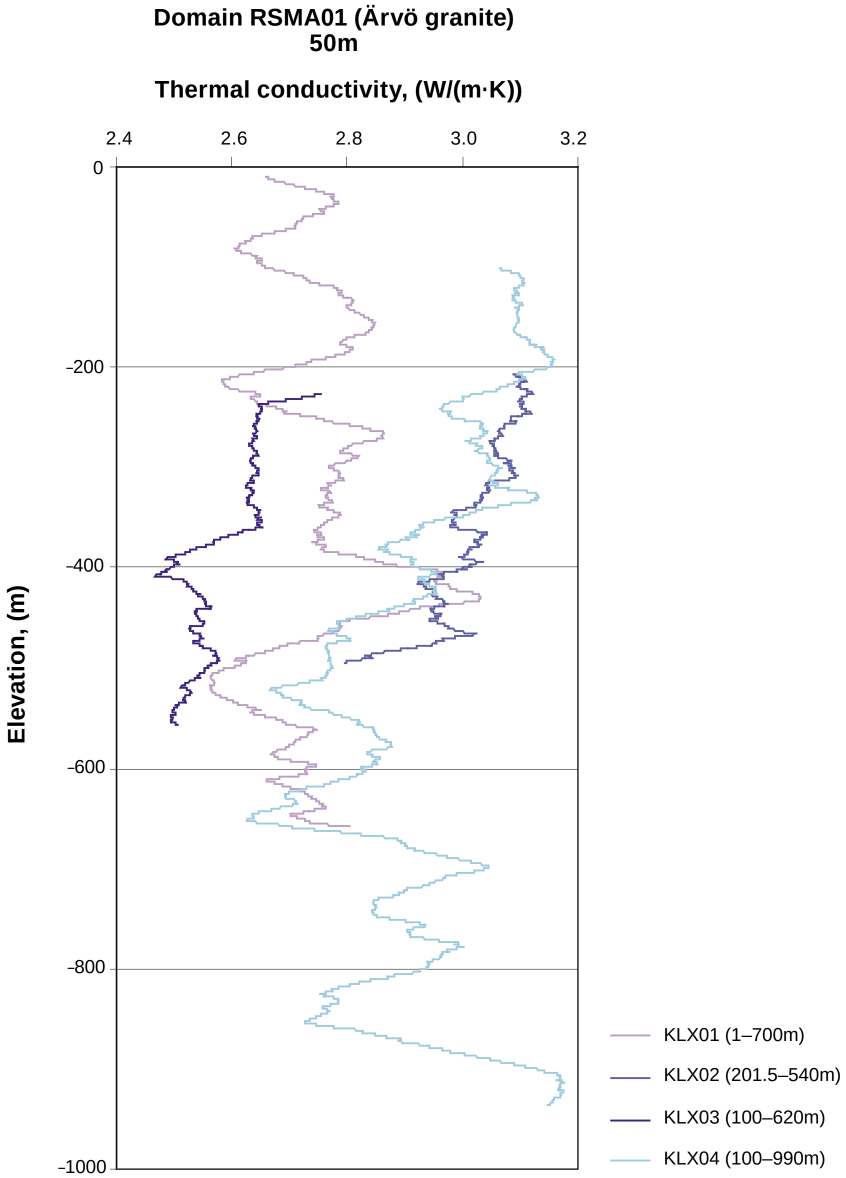

Figure 5-14. *Modelling results of borehole sections for domain RSMA. Thermal conductivity values are moving geometrical mean calculations over 50 m long sections (moving average). The results are based on only one realisation.*

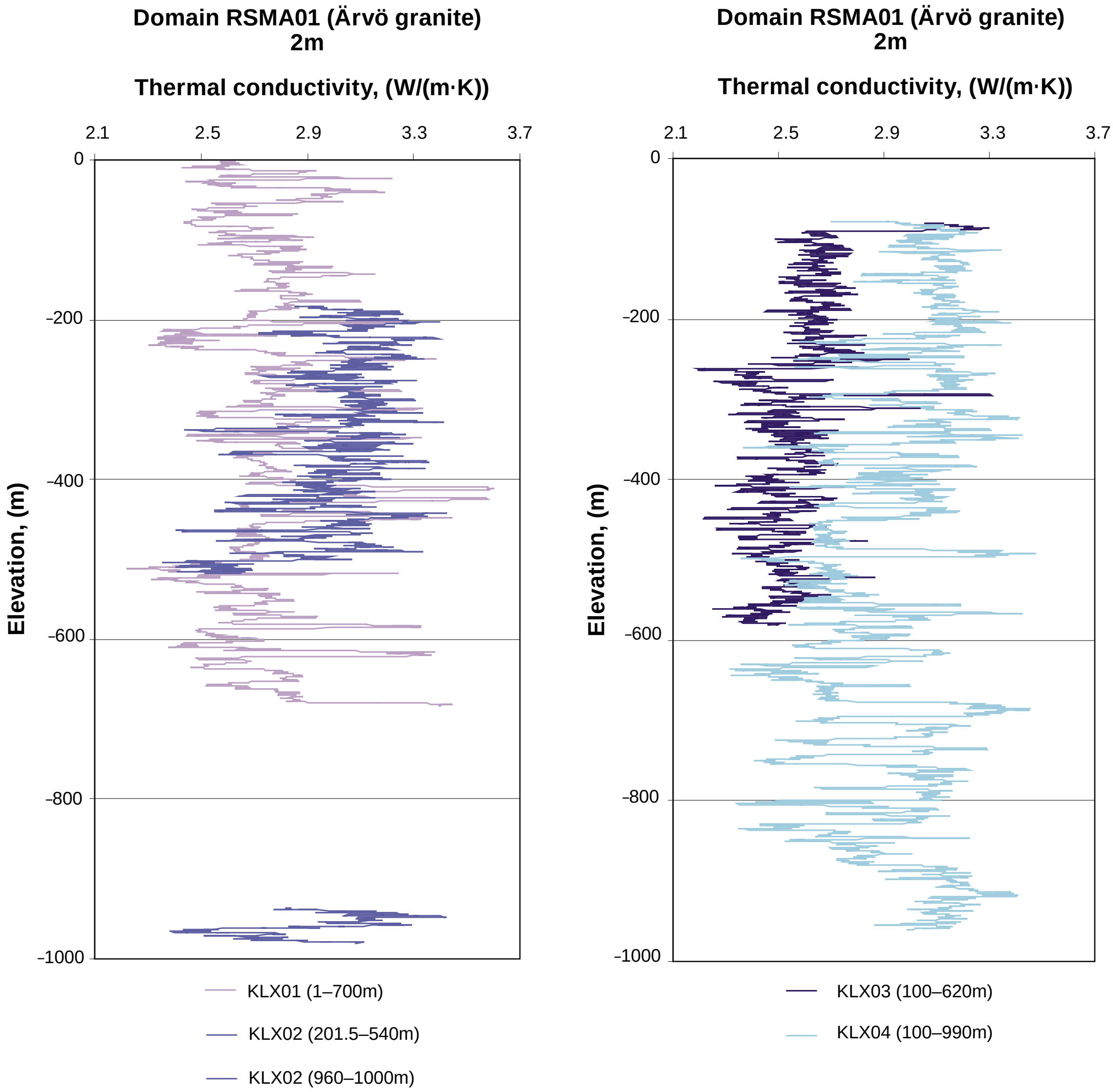

Figure 5-15. *Modelling results of borehole sections for domain RSMA. Thermal conductivity values are moving geometrical mean calculations over 2 m long sections (moving average). The results are based on only one realisation.*

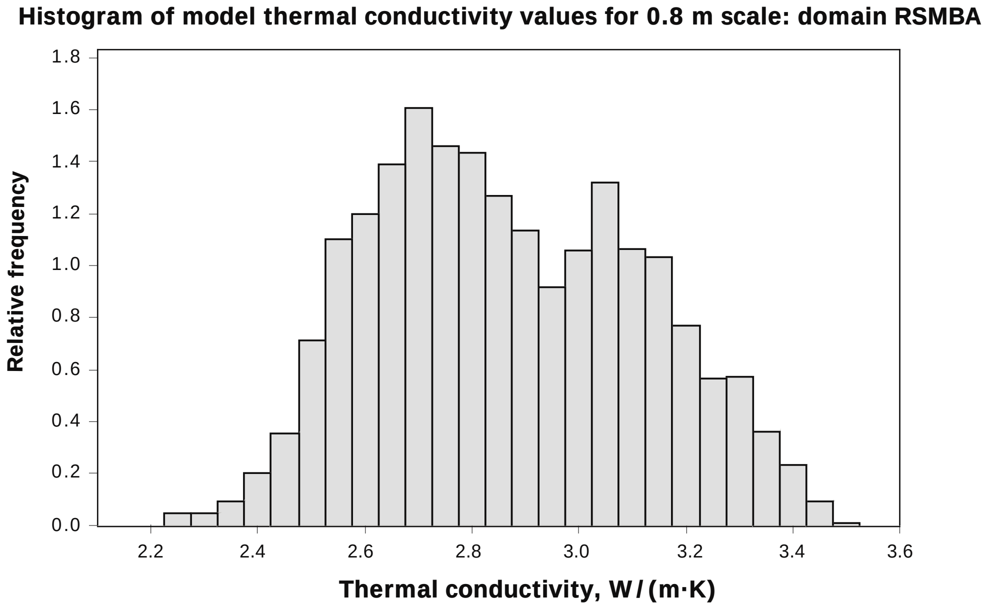

Figure 5-16. *Histogram of thermal conductivities for domain RSMBA at the 0.8 m scale using the base approach.*

Table 5-10. Modelling results for domain RSMBA with mean and standard deviation of the thermal conductivity (W/(m·K)) for 0.8 m scale and rock type distributions in percent.

	Domain RSMBA (based on borehole interval 540–960 m in KLX02)		
Rock name	**Percentages of rock types**		
Ävrö granite (501044)	57.9		
Fine-grained dioritoid (501030)	32.2		
Quartz monzodiorite (501036)	0		
Pegmatite (501061)	0.1		
Diorite/gabbro (501033)	0		
Fine-grained diorite-gabbro (505102)	7.9		
Granite (501058)	0		
Fine-grained granite (511058)	1.9		
	Thermal conductivity, W/(m·K)		
	0.1 m scale	**0.8 m scale**	**2 m scale**
Mean	2.88	2.87	2.86
Std dev	0.377	0.251	0.220

The changes in mean and, in particular, standard deviation that occur as a result of upscaling can be seen in Figure 5-17 and Figure 5-18, the differences being greatest between 0.1 and 2 m.

Figure 5-19 illustrates the modelled (according to the base approach) thermal conductivity plotted against elevation for the borehole section which constitutes domain RSMBA. The influence of subordinate rock type sections is clearly visible as spikes in the figures, but the variability within rock types may be underestimated according to the base modelling approach.

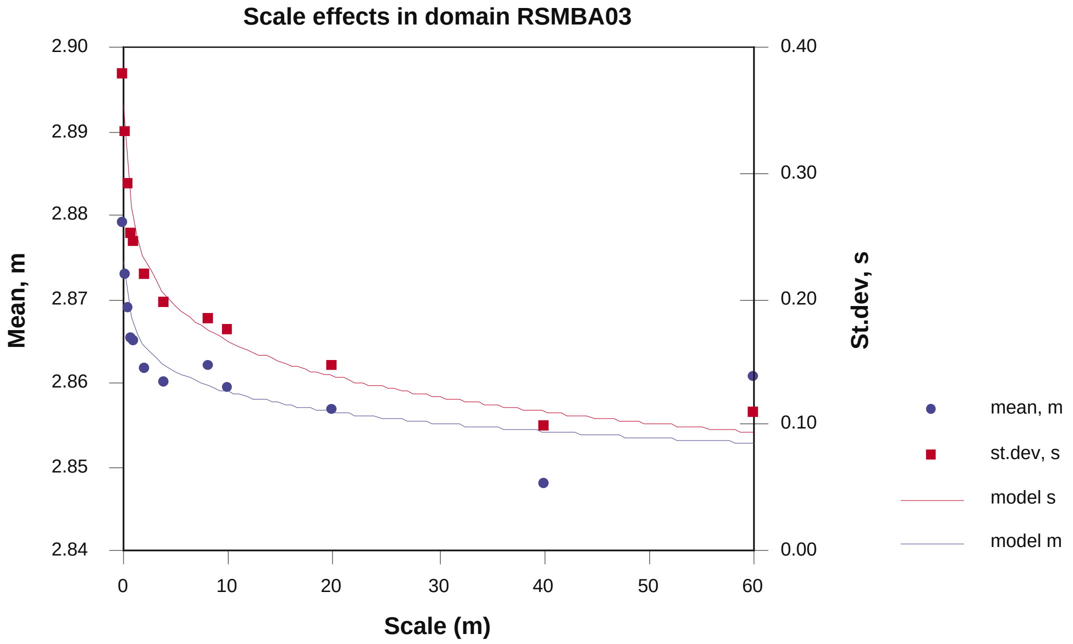

Figure 5-17. Modelling results of thermal conductivity for domain RSMBA: scale dependence (0.1 to 60 m) of mean and standard deviation. Logarithmic curves fitted to data.

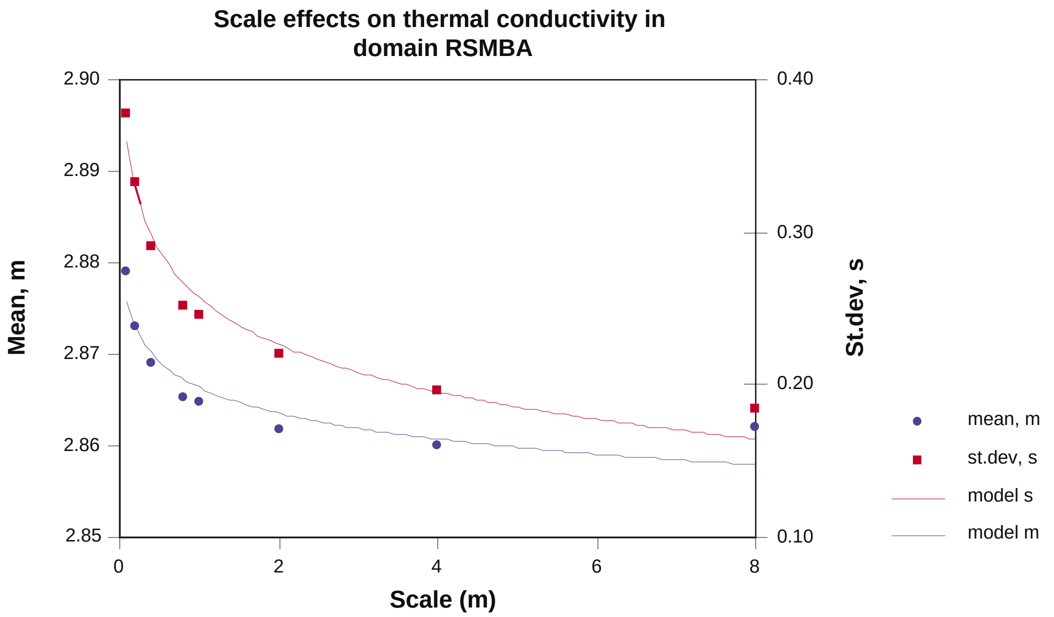

Figure 5-18. Modelling results of thermal conductivity for domain RSMBA: scale dependence (0.1 to 8 m) of mean and standard deviation. Logarithmic curves fitted to data.

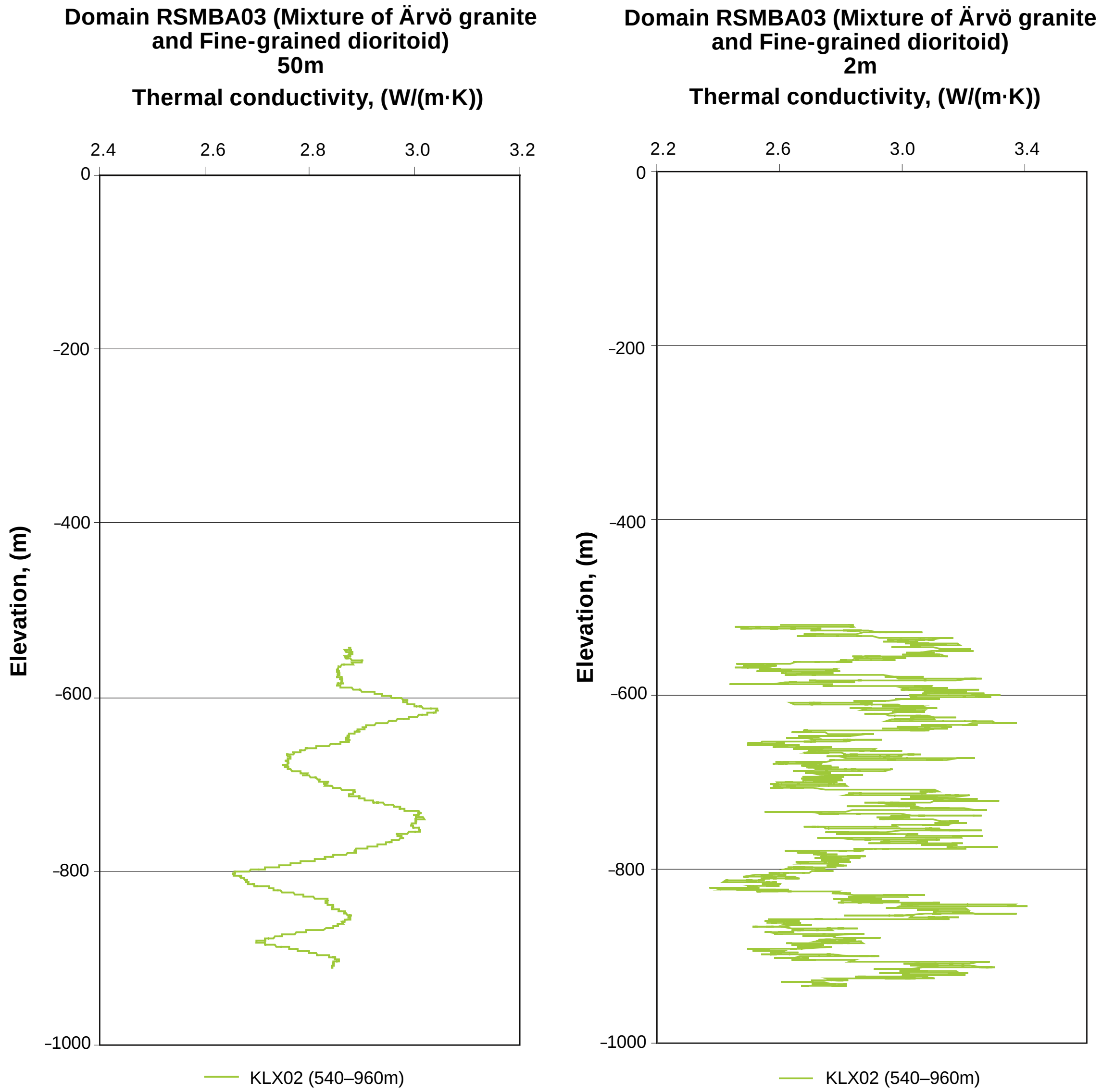

Figure 5-19. *Modelling results of borehole sections for domain RSMBA. Thermal conductivity values are moving geometrical mean calculations over 2 and 50 m long sections (moving average respectively). The results are based on only one realisation.*

Domain RSMD, Quartz monzodiorite

The dominant rock type in domain RSMD is quartz monzodiorite (501036). The domain is represented by a 380 m long borehole section (620–1,000 m) in KLX03 of which quartz monzodiorite comprises 84%, see Table 5-11. Since Ävrö granite constitutes only 2.5% of this domain, most of the thermal conductivities are derived from the distributions models (PDF) for the rock types present. Modelling results for the domain at the 0.8 m scale are presented in Table 5-11 and Figure 5-20. The data distribution is characterised by a relatively low standard deviation and a long tail towards higher values. Except for Ävrö granite, spatial variability within the rock types comprising this domain has not been taken into account. The resulting variance includes variability due to rock type changes in the boreholes ("between rock type" variability) but the variability within each rock type is effectively and rapidly reduced when the scale is increased because of the random assignment of thermal conductivity values. Thus the modelling approach adopted for domain RSMD underestimates the variance at the 0.8 m scale.

Table 5-11. Modelling results for the domain RSMD with mean and standard deviation of the thermal conductivity (W/(m·K)) for 0.8 m scale and rock type distributions in percent.

	Domain RSMD (based on borehole interval 620–1,000 m in KLX03)		
Rock name	**Percentages of rock types**		
Ävrö granite (501044)	2.5		
Fine-grained dioritoid (501030)	0.7		
Quartz monzodiorite (501036)	84.4		
Pegmatite (501061)	1.1		
Diorite/gabbro (501033)	0		
Fine-grained diorite-gabbro (505102)	7.2		
Granite (501058)	0.6		
Fine-grained granite (511058)	3.6		
	Thermal conductivity, W/(m·K)		
	0.1 m scale	**0.8 m scale**	**2 m scale**
Mean	2.71	2.70	2.70
Std dev	0.228	0.128	0.103

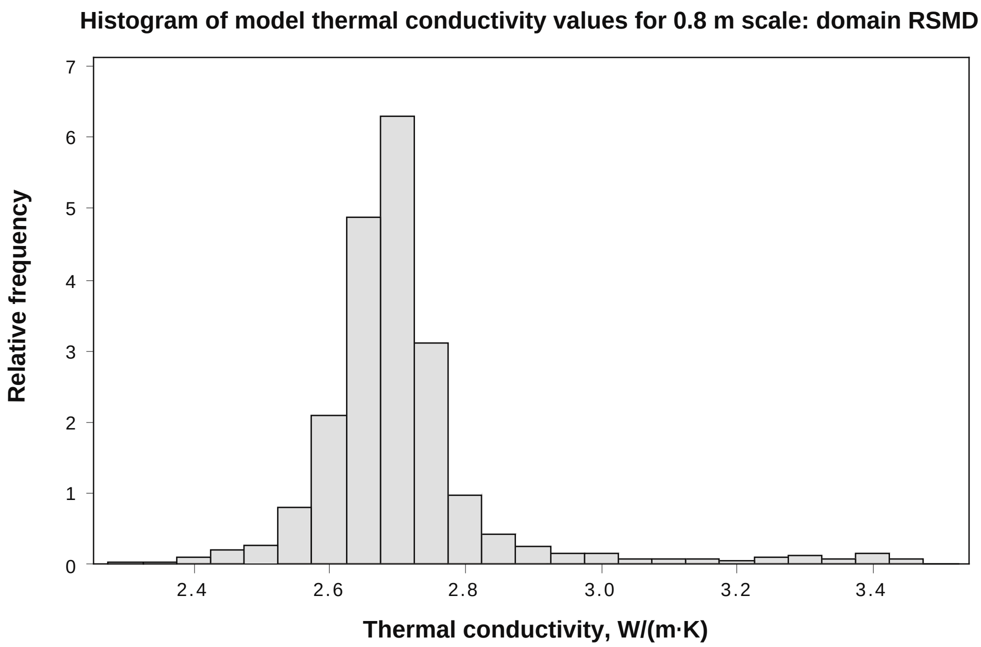

***Figure 5-20.** Histogram of thermal conductivities for domain RSMD at the 0.8 m scale using the base approach.*

The changes in mean and, in particular, standard deviation that occur as a result of upscaling can be seen in Figure 5-21 and Figure 5-22, the differences being greatest between 0.1 and 2 m.

Figure 5-23 illustrates the modelled (according to the base approach) thermal conductivity plotted against elevation for the boreholes section which constitutes the domain RSMD. The influence of subordinate rock type sections is clearly visible as spikes in the figures, but the variability within rock types may be underestimated according to the base modelling approach.

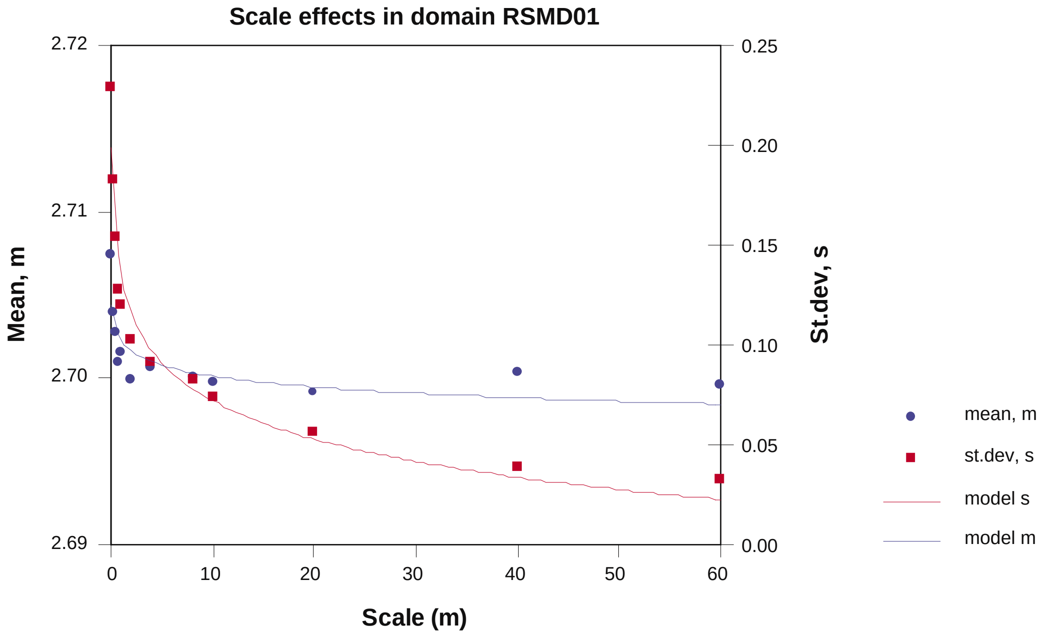

Figure 5-21. *Modelling results of thermal conductivity for domain RSMD: scale dependence (0.1 to 60 m) of mean and standard deviation. Logarithmic curves fitted to data.*

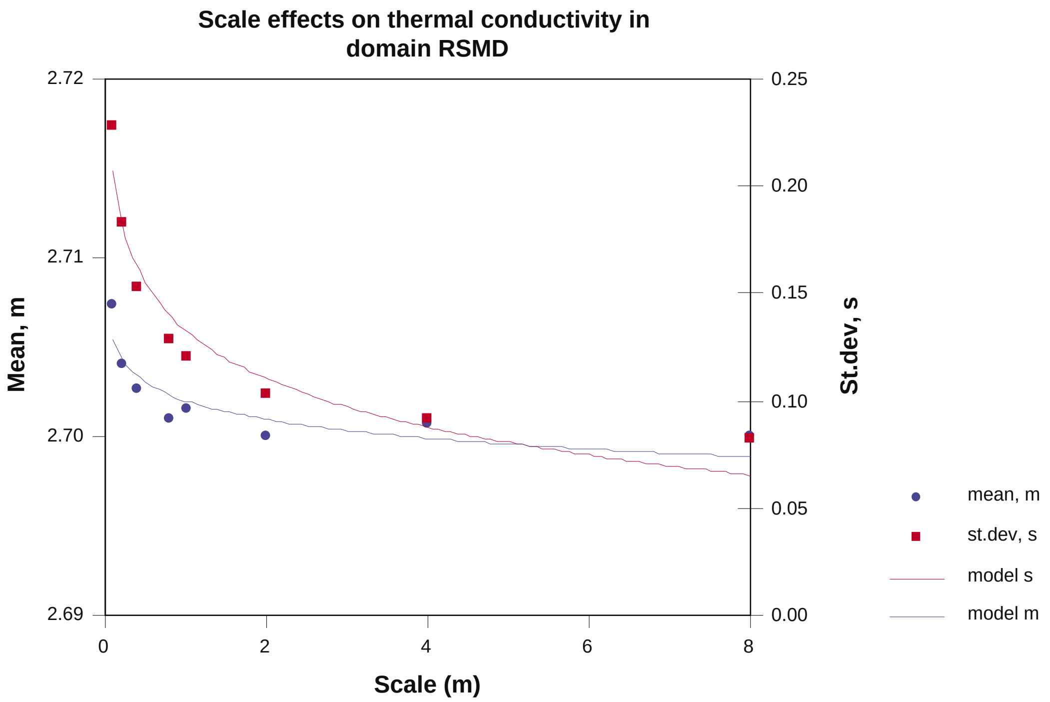

Figure 5-22. *Modelling results of thermal conductivity for domain RSMD: scale dependence (0.1 to 8 m) of mean and standard deviation. Logarithmic curves fitted to data.*

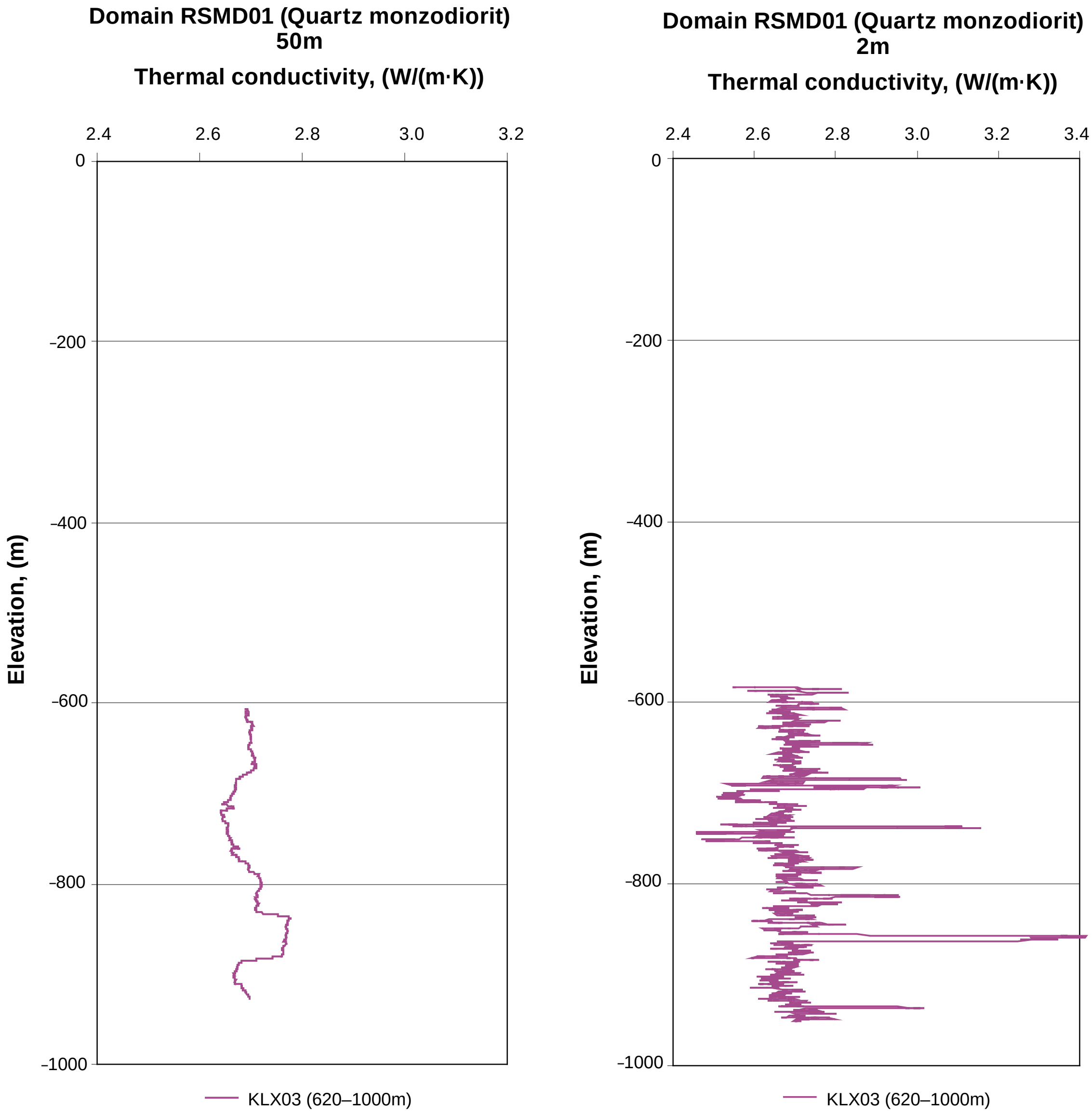

Figure 5-23. *Modelling results of borehole sections for domain RSMD. Thermal conductivity values are moving geometrical mean calculations over 2 and 50 m long sections (moving average) respectively. For domain RSMD the spatial variability within rock types other than for Ävrö granite is not considered. Consequently the variability is underestimated for this domain. The results are based on only one realisation.*

Domain RSME, Diorite/gabbro

Domain RSME is a small domain found in the north-eastern corner of the Laxemar subarea. The RSME domain is dominated by diorite/gabbro (501033). There are no boreholes intercepting this domain so the rock type composition of 95% diorite/gabbro (501033) and 5% fine-grained granite (511058) has been based on estimates from surface geological mapping /Wahlgren et al. 2005a/. The rock type models for diorite/gabbro and fine-grained granite are based on small numbers of samples, for which in most cases thermal conductivity has been calculated from mineral composition. Because of the lack of borehole data, the approach applied to the domains described above cannot be applied. Therfore, a simplified approach based on Monte Carlo simulation is used in modelling this domain. The results are presented in Table 5-12 and Figure 5-24.

Table 5-12. Thermal conductivity (W/(m·K)) of domain RSME (diorite/gabbro). Modelling results from Monte Carlo simulation with upper and lower 2.5 percentiles. Note that the scale is < 0.1 m; no upscaling performed.

Domain	Mean	Std dev
RSME	2.45	0.29

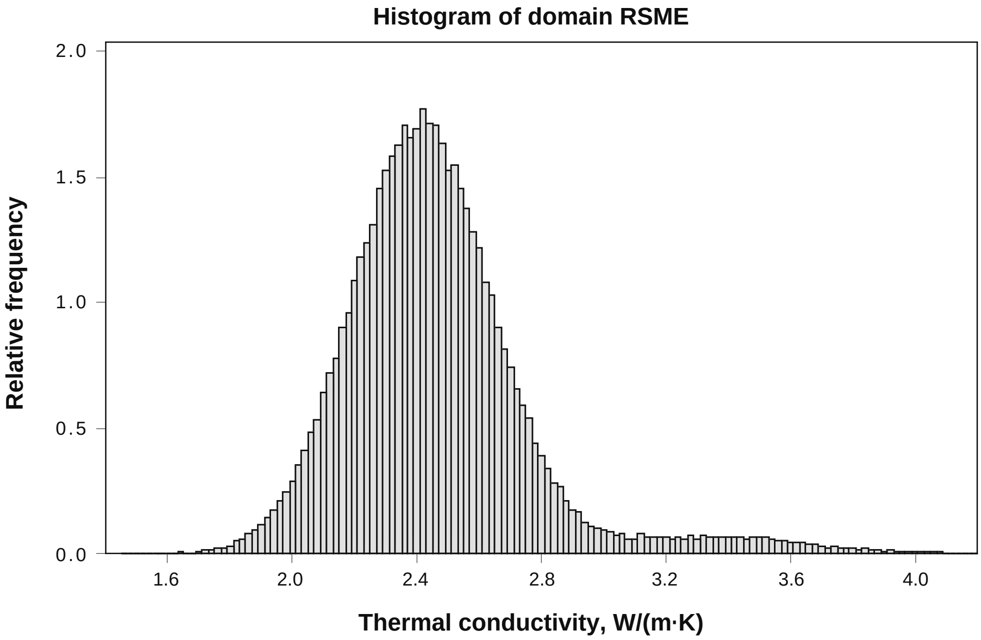

Figure 5-24. *Histogram of thermal conductivities for domain RSME from Monte Carlo simulation.*

The approach used for this domain does not take any account of variance reduction due to upscaling. Therefore, the quoted standard deviation most likely overestimates the dispersion at a larger scale for this domain since the data on which the rock model PDFs are based are for the TPS scale (dm scale). The same argument holds for the upper and lower 2.5 percentiles. However, there are large uncertainties associated with both the estimated rock type composition of the domain and the rock type models.

Domain RSMM, Mixed zone with large fraction of diorite/gabbro

The rock type distribution for domain RSMM is based on results from surface geological mapping since this data was considered to best represent the present-day knowledge of the domain as a whole /Wahlgren et al. 2005a/. Borehole KLX03 which intercepts this domain is not considered representative of the rock type composition. The major rock types in domain RSMM (see Table 5-5) are diorite/gabbro (12%), Ävrö granite (53%) and quartz monzodiorite (27%) /Wahlgren et al. 2005a/. Because of the lack of borehole data a simplified approach based on Monte Carlo simulation is used in modelling this domain. The results are presented in Table 5-13, Figure 5-25 and Figure 5-26.

Two alternatives are presented since Ävrö granite can be modelled in different ways. In alternative 1, Ävrö granite has been modelled using a rock type model (PDF) based on a normal distribution from TPS measurements, see 4.6.6. Problems associated with this approach are 1) assuming a normal distribution is evidently inadequate in describing this rock type (as mentioned previously the Ävrö granite is characterised by a bimodal distribution), and 2) the entire variability within the Ävrö granite is, based on the data available, unlikely to be present in domain M. Evidence from density logging in borehole KLX03 (Figure 4-22) and from surface samples of Ävrö granite in southern Laxemar (Figure 4-7) indicates that the low thermal conductivity mode is dominant in the M domain. Replacing the rock type model based on TPS measurements with a model based on results of density logging in KLX03 produces quite a different mean thermal conductivity (alternative 2). The results of these two alternative approaches are presented in Table 5-13.

Again, the quoted parameters of dispersion are probably overestimates at the 0.8 m scale, since the data on which the rock model PDFs are based are for the TPS scale (dm scale). Variance reduction due to upscaling is not considered. The estimated rock type composition of the domain is also uncertain.

Because of its heterogeneity, the domain has several "subvarieties" with different thermal properties. For example, borehole interval 100 to 800 m in KLX03 has been divided into a section dominated by Ävrö granite (RSMM(A)) and a section dominated by quartz monzodiorite (RSMM(D)). However, because of the low amount of diorite/gabbro, these sections cannot be considered representative of the domain. Instead, they can be interpreted as two of perhaps several varieties in this domain. These have been modelled separately and give mean values of 2.57 W/(m·K) for the M(A) type and 2.69 W/(m·K) for the M(D) type.

Table 5-13. Thermal conductivity (W/(m·K)) of domain RSMM. Modelling results from Monte Carlo simulation with upper and lower 2.5 percentiles. Note that the scale is < 0.1 m; no upscaling performed.

	Mean	Std dev	Comment
Alt. 1	2.78	0.34	Rock type model for Ävrö granite based on TPS measurments
Alt. 2	2.58	0.22	Rock type model for Ävrö granite based on density loggings in KLX03

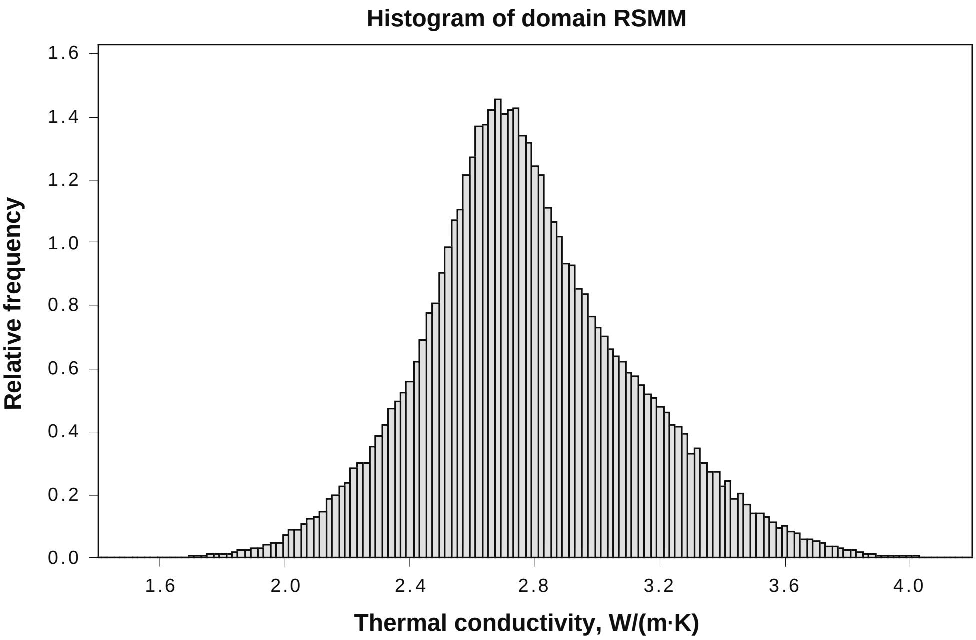

Figure 5-25. *Histogram of thermal conductivities for domain RSMM from Monte Carlo simulation (alternative 1).*

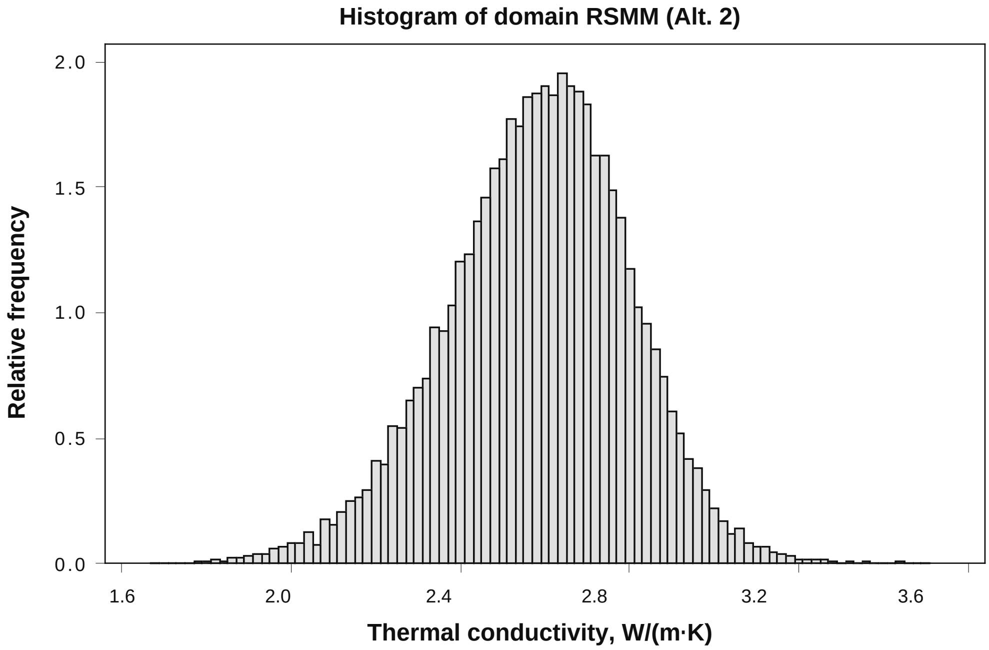

Figure 5-26. *Histogram of thermal conductivities for domain RSMM from Monte Carlo simulation (alternative 2).*

Summary of domain modelling according to base approach

In Table 5-14, the mean thermal conductivity together with standard deviations and upper and lower tails (defined as 0.5, 2.5 and 97.5 percentiles) are presented for 0.8 m scale for three domains. It should be noted that the emphasis is placed on lower tail percentiles of the distributions as it is these that are critical for design purposes. In work on thermal modelling of the Simpevarp subarea /Sundberg et al. 2005b/ the 2.5^{th} and 97.5^{th} percentiles of model thermal conductivity values were estimated under the assumption of normal distribution. However, histograms and probability plots (Appendix B) of modelled conductivity values for domains RSMA, RSMBA, and RSMD indicate that the data populations for the different domains cannot be assumed to be normal. Nor can transformation make them approximately normal. Therefore, percentiles can be estimated more accurately using nonparametric percentile estimation /Mac Berthouex and Brown 2002/, which does not require a distribution to be known or assumed but can be applied to any data set. In Table 5-14 results of both methods of estimating the upper and lower tails are shown. Taking the 2.5 and 97.5 percentiles, 95% of the data values fall within these limits. For domain RSMA, the 95% upper and lower confidence limits for the 0.5 and 2.5 percentiles have been estimated, using a method according to /Gilbert 1987/, as ± 0.02 and ± 0.05 respectively.

For domains RSMA, RSMBA and RSMD, when the data is assumed to be normally distributed, both the 0.5 and 2.5 percentiles are lower by between 0.06 and 0.14 W/(m·K) than estimates calculated directly from the data set. These differences will be seen to be of importance for approximating lower 0.5 and 2.5 percentiles from the results of the alternative approaches, see 5.5.1.

Table 5-15 summarises the mean thermal conductivities for domains RSMM and RSME. The quoted standard deviation most certainly overestimates the dispersion at a larger scale for these domains since the data on which the rock model PDFs are based, are for the TPS scale (dm scale). For the same reason, the estimated 0.5 and 2.5 percentiles are unreasonably low at a scale relevant to the canister. For domain RSMM, the interesting point to note

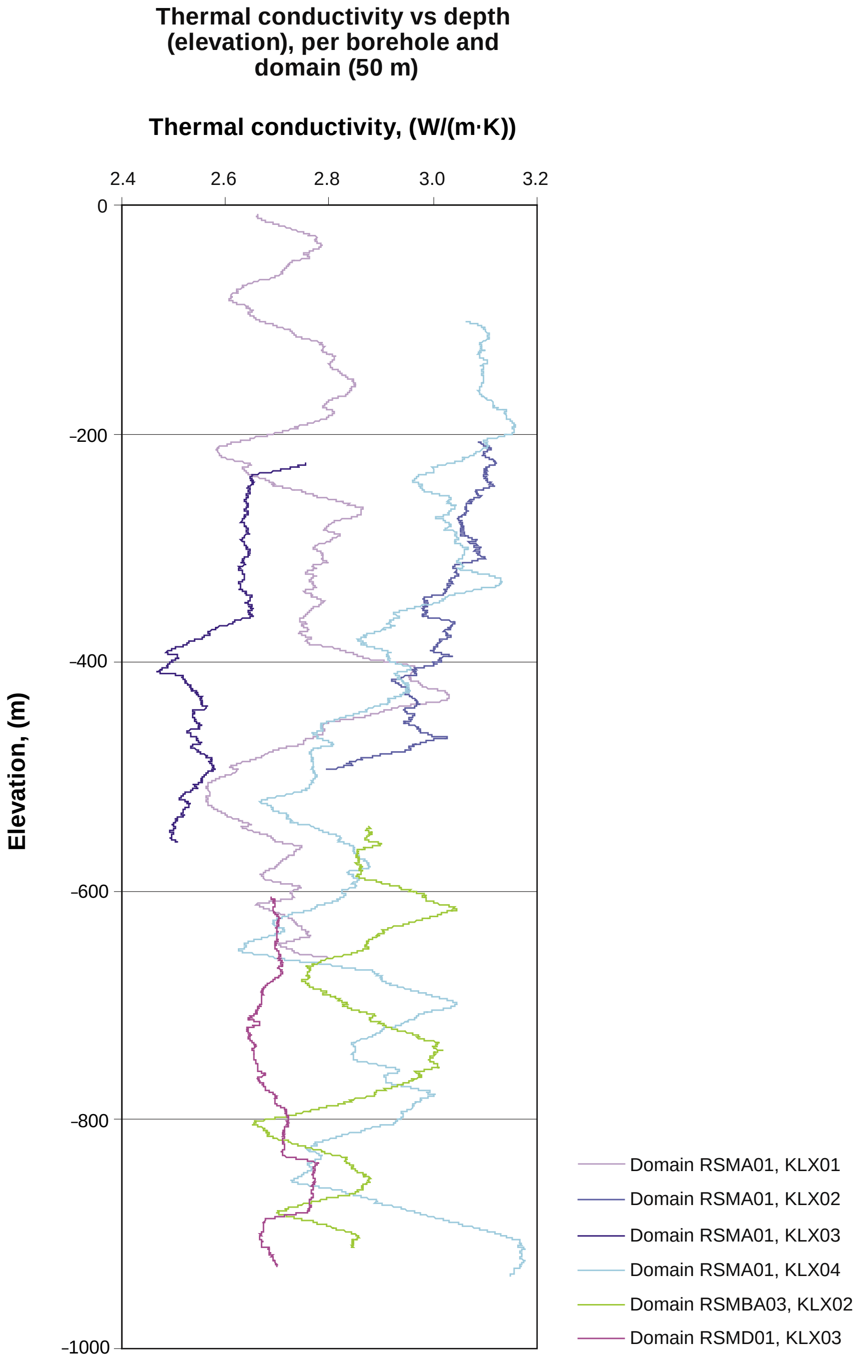

Figure 5-27. *Visualisation of changes in thermal conductivity with depth for borehole sections for three domains (RSMA, RSMBA and RSMD). Thermal conductivity is expressed as moving geometrical mean calculations over 50 m long sections. For domain RSMD the spatial variability within rock types other than for Ävrö granite is not considered. Consequently the variability is underestimated for this domain. The results are based on only one realisation.*

Table 5-14. Thermal conductivity (W/(m·K)) modelling results at 0.8 m scale for domains RSMA, RSMBA and RSMD. Upper and lower tails (percentiles) are calculated from the modelled data distribution according to base approach (1) and assuming a normal distribution (2).

Domain	Mean	Std dev	0.5 percentile (1)	0.5 percentile (2)	2.5 percentile (1)	2.5 percentile (2)	97.5 percentile (1)	97.5 percentile (2)
RSMA	2.821	0.281	2.238	2.097	2.352	2.270	3.365	3.372
RSMBA	2.865	0.251	2.342	2.218	2.446	2.373	3.347	3.357
RSMD	2.701	0.128	2.428	2.371	2.522	2.450	3.104	2.952

Table 5-15. Thermal conductivity (W/(m·K)) modelling results from Monte Carlo simulation for domains RSME and RSMM. The scale is < 0.1 m. No upscaling has been implemented, which implies variability overestimated for larger scales.

Domain	Mean	Std dev	0.5 percentile	2.5 percentile	97.5 percentile
RSME	2.45	0.29	1.85	1.98	3.22
RSMM (Alt. 1)	2.78	0.34	1.98	2.15	3.51
RSMM (Alt. 2)	2.58	0.22	1.98	2.13	2.98

here is that despite the large difference in the mean given by the two alternatives, both yield similar 0.5 and 2.5 percentiles. However, the mean from alternative 2 is considered more reasonable (see above) than that from alternative 1, since it thought that the latter overestimates the thermal conductivity of this domain, see section 5.3.2.

5.4.3 Approach 1: Addition of simulated within rock variability from domain RSMA

This approach has been applied to domain RSMD, which is dominated by quartz monzodiorite. Variance caused by spatial variability within Ävrö granite was estimated for domain RSMA according to the method outlined in 5.3.3. The "within rock type" variance for Ävrö granite in domain RSMA is then added to the "between rock type" variance calculated for domain RSMD. The results of this approach are presented in Table 5-16.

According to this approach the standard deviation of domain RSMD is similar to that of domain RSMA and RSMBA. This is most probably an overestimation of the variance for domain RSMD since Ävrö granite (which RSMA and RSMBA mainly consists of) is the rock type with the largest variation in composition and, therefore, also the largest dispersion in thermal conductivity.

5.4.4 Approach 2: Extrapolation of spatial variability

As described above, when modelling domain RSMA (dominated by Ävrö granite) and RSMBA (mixture of Ävrö granite and fine-grained dioritoid) according to the base approach, "within rock type" variability was not considered for the whole borehole length. By randomly replacing thermal conductivity values estimated from density logging with random PDF values it is possible to study the effect of ignoring this type of spatial variability for part of the borehole.

Figure 5-28 illustrates an extrapolation of the standard deviation for the scale 0.8 m as a function of the percentage of spatial data used in the modelling of domain RSMA. If the spatial variability is considered to its full extent, the standard deviation of domain RSMA at 0.8 m scale is estimated to be 0.295 W/(m·K) (point C in Figure 5-28), which corresponds to a variance of 0.087 $(W/m·K)^2$. This can be compared to a standard deviation of 0.281 when 81.5% of the spatial variability is considered (point B in Figure 5-28). The variance contribution due to spatial variability within rock types is then 0.056 $(W/m·K)^2$, which differs from 0.048 $(W/m·K)^2$ estimated by the base approach, see Table 5-21.

The same approach can be applied to domain RSMBA. For convenience the same curve as was used for domain RSMA has been applied to calculate the standard deviation when the total spatial variation is considered. The difference in variance between 55.5% (the proportion of the borehole for which density loggings were employed) and 100% is determined and then added to the variance determined in the base approach. The resulting variance for domain RSMBA is 0.085 $(W/m·K)^2$ corresponding to a standard deviation of 0.291 W/(m·K).

It is reasonable to assume that this method of correction overestimates the total variance since the spatial variation of rock types other than Ävrö granite (501044) within domains RSMA and RSMBA is probably significantly smaller, a factor which is not considered in the correction.

Table 5-16. Thermal conductivity (W/(m·K)) modelling results at 0.8 m scale for domain RSMD.

Scale (m)	Mean	Std dev	Std dev (within rock variability from RSMA included)
RSMD (0.8 m)	2.701	0.128	0.255

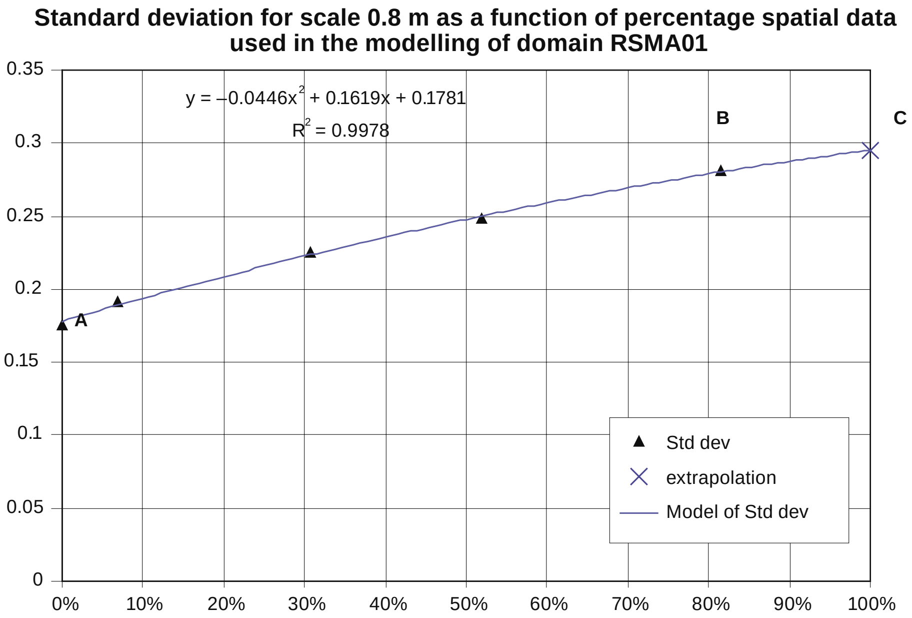

__Figure 5-28.__ Extrapolation of standard deviation for thermal conductivity at scale 0.8 m as a function of the percentage of spatial data used in the modelling of domain RSMA. At point A, all data are randomly assigned from rock types PDF:s without consideration of spatial variability within Ävrö granite. Point B corresponds to 81.5% of the values estimated from density loggings and thus considering spatial variability. Point C is extrapolated and corresponds to 100% spatial data values, assuming the same spatial variability within all rock types as in Ävrö granite.

5.4.5 Approach 3: Subtraction of small scale variability

In the third approach, the small-scale variability within Ävrö granite in RSMA at the scale of interest is subtracted from the total variability of the same rock type. Variograms presented in Figure 5-5 are used to estimate the small-scale variance of Ävrö granite, the dominant rock type in domain RSMA.

Table 5-17 illustrates rough estimations of the variance at two different scales based on variograms and PDF:s, and also the variance residual after averaging to the desired scale.

A modification of this approach is used to evaluate the spatial variability within domain RSMD. It uses the variance reduction within Ävrö granite as a result of upscaling expressed as a percentage of the total sample variance for this rock type. For scale 0.8 m the variance reduction is estimated at 37% (Table 5-17). Assuming that the variance reduction as a result of upscaling within quartz monzodiorite (domain RSMD) is of the same relative magnitude, the residual variance within this rock type can also be estimated (Table 5-18). This assumption is considered reasonable since both Ävrö granite and quartz monzodiorite are granitoid rocks with similar grain size.

There is a reason to believe that this approach may overestimate the variance at domain level because the variance within subordinate rock types is probably less than for the dominant rock type (Ävrö granite).

Table 5-17. Estimated variances $(W/(m\cdot K))^2$ in different scales based on variograms of the Ävrö granite (501044) in domain RSMA. Presented values are mean values of data from four boreholes KLX01, KLX02, KLX03 and KLX04.

	Scale 0.8 m		Scale 2 m	
	Variance	Std dev	Variance	Std dev
Total variance within the rock type	0.098		0.098	
Small scale variance	0.036		0.041	
Spatial variance left after equalization to desired scale	0.062	0.25	0.057	0.24

Table 5-18. Estimated variances $(W/(m\cdot K))^2$ of quartz monzodiorite for 0.8 m scale based on variograms of the Ävrö granite (501044) in domain RSMA.

	Scale 0.8 m	
	Variance	Comment
Total variance within the rock type	0.0196	Sample variance for quartz monzodiorite
Small scale variance	0.0073	37% of sample variance
Spatial variance left after equalization to desired scale	0.0123	

5.4.6 Approach 4: Upscaling of "within rock type" variability

In the thermal modelling work for Simpevarp 1.2 a rough estimate of the spatial variability within rock type fine-grained dioritoid (501030) was determined from TPS measurements. For Ävrö granite (501044) values calculated from density loggings from four boreholes within Laxemar subarea have been used. The calculated within rock-type variances as a function of scale are presented in Figure 5-29 for Ävrö granite and fine-grained dioritoid. These results are applied to the domains in the Laxemar subarea.

The total variance estimated for each domain is presented in Table 5-19.

For domain RSMBA there are two dominant rock types. Therefore, the within rock-type variance is estimated slightly differently, as a weighted sum of the spatial variance for the two dominant rock types, where the weighting factors are the fractions of each rock type in the domain. The weighting of variances in this way, although not entirely permissible in theory, is a rough attempt at an approximation of the spatial variability within rock types.

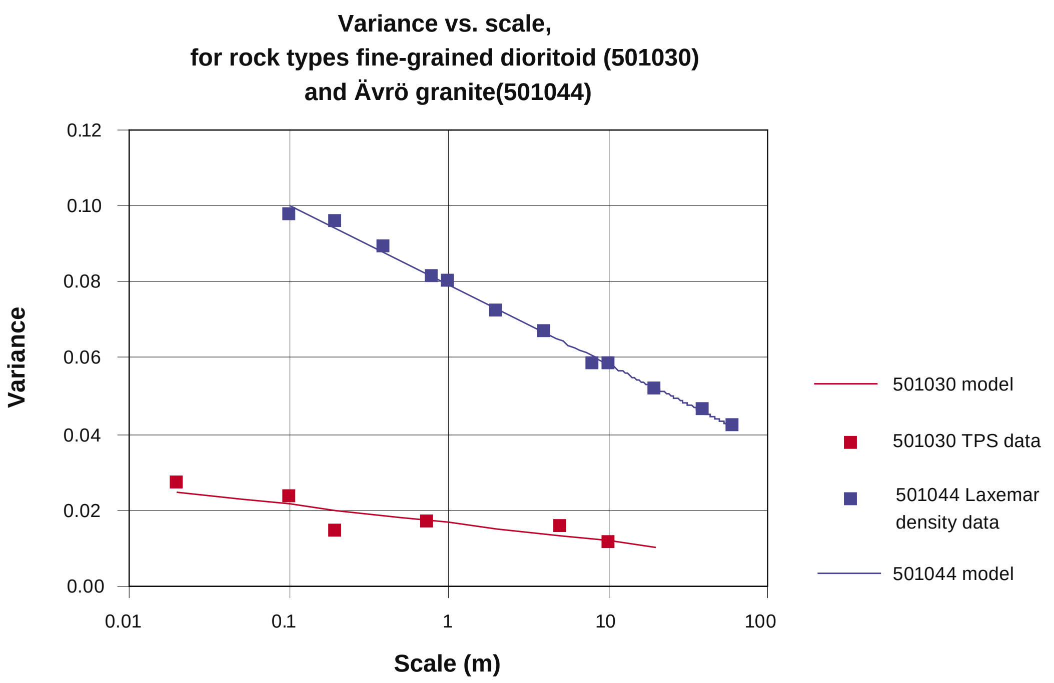

Figure 5-29. *Comparison between "within rock type" variability for fine-grained dioritoid (501030) and Ävrö granite (501044). Note that data for 501030 are sparse and based on 26 TPS measurements from two boreholes in Simpevarp, while data for 501044 are based on calculated values determined from density loggings from four boreholes within domain RSMA in Laxemar subarea.*

Table 5-19. Variances $(W/(m \cdot K))^2$ for the 0.8 m scale for three different domains according to approach 4.

Rock type	Scale 0.8 m RSMA (501044)	RSMBA (501044+ 501030)	RSMD (501036)
Variance (V_1)	0.031	0.026	0.017
Variance (V_2), Figure 5-29	0.082	0.059[1]	0.030[2]
Variance (V_{tot})	0.113	0.085	0.047
Std dev_{tot}	0.336	0.292	0.217

[1] Internal spatial variance within the rock types in the domain calculated with a composition of 64% Ävrö granite and 36% fine-grained dioritoid (0.64·0.082+0.36·0.018 = 0.059), see Table 5-4.

[2] Internal spatial variance within the rock types in the domain calculated with a composition of 84% Quartz monzodiorite (variance at sample scale = 0.020) and 16% Ävrö granite (0.84·0.020+0.16·0.082 = 0.030). Domain D consist of only 2–3% Ävrö granite, but so as not to underestimate the variance of the minor rock types in the domain the variance of Ävrö granite at scale 0.8 m is used.

In the absence of scale-related data for quartz monzodiorite, this rock type can be assigned a value for within-rock variance derived from the measurement data set, which represents a scale less than 1 dm. Again, the within rock-type variance is estimated as a weighted sum of the spatial variance for the dominant rock type plus the variance for the remaining subordinate rock types assuming an Ävrö granite composition. This is a conservative approach and most likely overestimates the variance.

It is not easy to assess whether this approach under- or overestimates the total variance for the domain. There are several factors that may influence this, such as the spatial variability in subordinate rock types compared to dominant rock type. In addition, the within rock-type variance for fine-grained dioritoid in Figure 5-29 is rather uncertain due to relatively few measurements and questions of representativeness. Still, it is believed that this approach gives a quite reasonable estimate of the variability compared to the other approaches, but a prerequisite is that a sufficient number of TPS measurements are available.

5.4.7 Heat capacity: Domain properties

Approach

Calculations of mean and upper and lower tails for frequency distributions of heat capacity have been performed by Monte Carlo simulation for four of the rock domains in the Laxemar subarea. The different rock types in the domains are weighted according to their relative abundance. Normal distribution models for rock types fine-grained dioritoid (501030), quartz monzodiorite (501036) and Ävrö granite (501044) are based on the data in Table 4-23. Other rock types have not been considered due to the unavailability of measurements. From the simulation, the mean, standard deviation in addition to 2.5th and 97.5th percentiles of data values have been calculated.

Results

The Monte Carlo simulations for the domains RSMA, RSMBA, RSMD and RSMM are presented in Figure 5-30, Figure 5-31, Figure 5-32 and Figure 5-33. The results are summarized in Table 5-20.

Observe that the above table is valid at 20°C. With increasing temperature the heat capacity increases considerably, see Table 4-24. The increase is approximately 25% per 100°C temperature increase for rock types Ävrö granite, quartz monzodiorite and fine-grained dioritoid. Thus the estimated change in heat capacity for domains RSMA, RSMBA, RSMD and RSMM is approximately 25% per 100°C temperature increase.

Table 5-20. Heat capacity MJ/(m^3·K) of domains RSMA, RSMBA, RSMD and RSMM with 2.5 and 97.5 percentiles.

Domain	Mean value	Std dev	2.5 percentile	97.5 percentile
RSMA	2.24	0.13	1.98	2.50
RSMBA	2.23	0.12	1.99	2.48
RSMD	2.29	0.12	2.06	2.52
RSMM	2.25	0.13	1.99	2.47

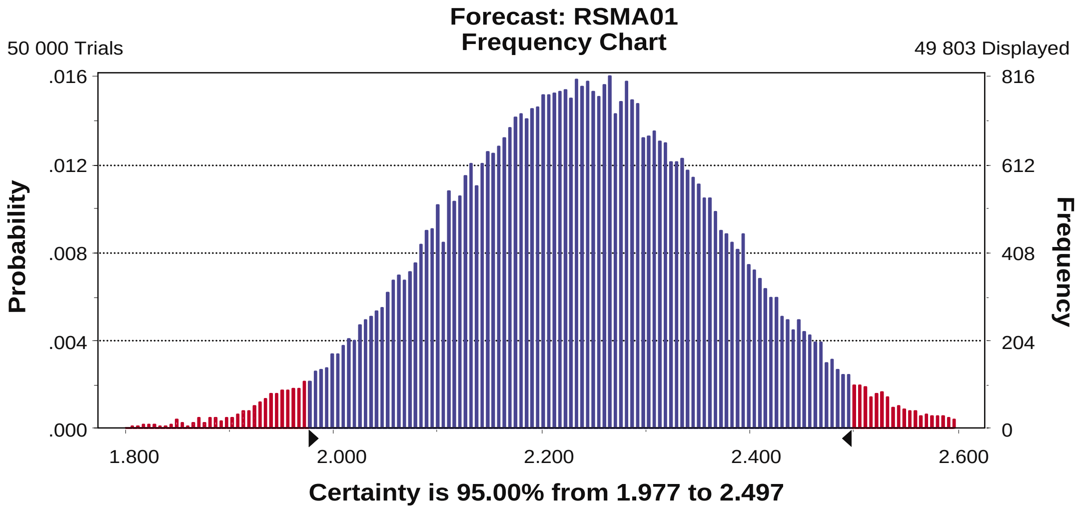

Figure 5-30. *Monte Carlo simulation results for the heat capacity of domain RSMA. 2.5 and 97.5 percentiles are marked with arrows.*

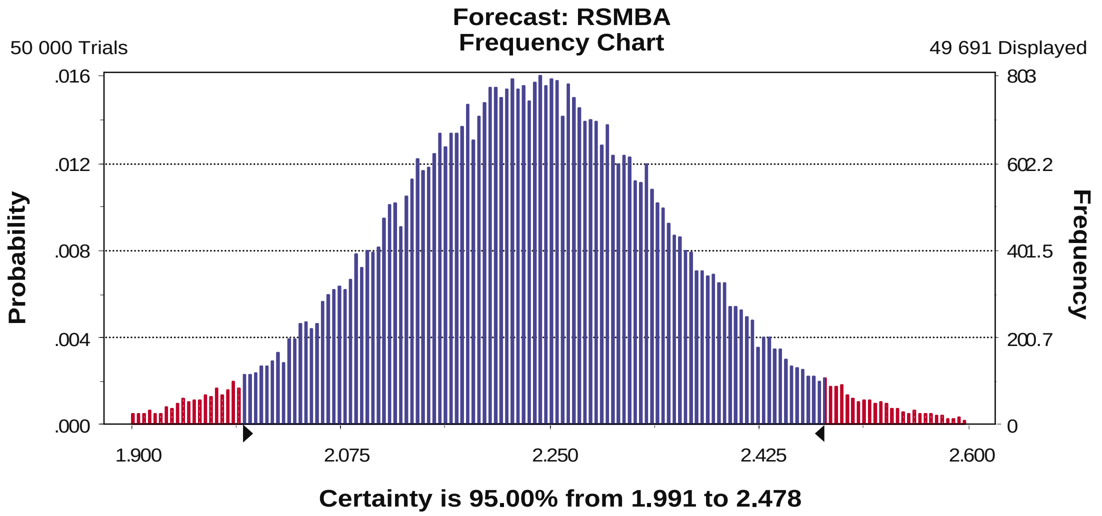

Figure 5-31. *Monte Carlo simulation results for the heat capacity of domain RSMBA03. 2.5 and 97.5 percentiles are marked with arrows.*

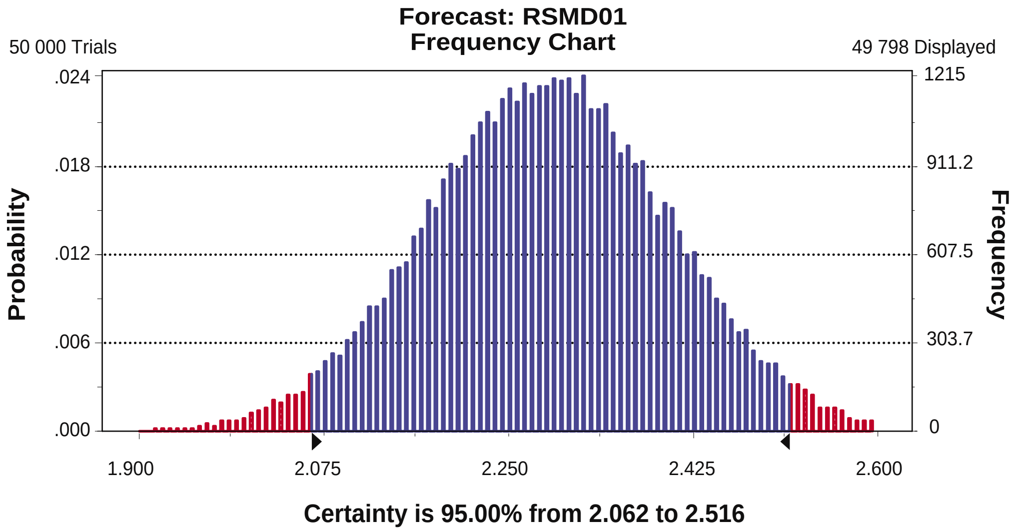

Figure 5-32. *Monte Carlo simulation results for the heat capacity of domain RSMD. 2.5 and 97.5 percentiles are marked with arrows.*

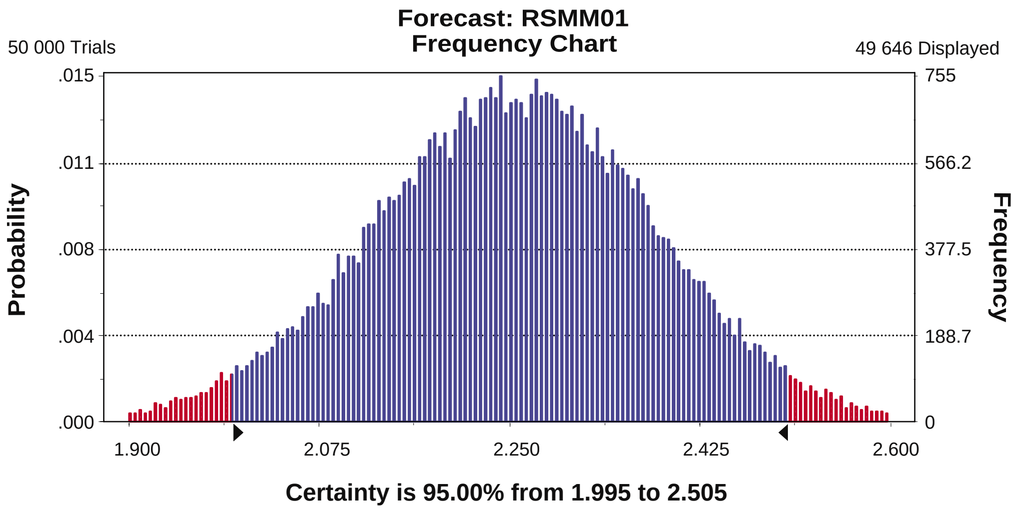

Figure 5-33. *Monte Carlo simulation results for the heat capacity of domain RSMM. 2.5 and 97.5 percentiles are marked with arrows.*

5.4.8 In situ temperature

The in situ temperature data derived from loggings might possibly reflect large scale spatial variability in thermal properties for the investigated area. In this site descriptive model version 1.2 of the Laxemar subarea, however, no modelling from temperature loggings has been done. The main reason for not modelling the temperature is that the temperature data is associated with a high degree of uncertainty for reasons mentioned in section 4.11, and discussed further in section 6.3.

5.5 Evaluation of domain modelling results

5.5.1 Mean thermal conductivity

Mean thermal conductivity for the domains are estimated according to the base approach. A summary of the mean thermal conductivity at domain level for the 0.8 m scale is presented in Table 5-21. The variation of the mean as a result of scale is small, however. Although thermal conductivities for domains RSMA and RSMBA are presented as means, it should be borne in mind that both domains display bimodal data distributions, see Figure 5-11 and Figure 5-16. For domain RSMM, see section 5.4.2, the result from alternative 2 is considered more reasonable than that from alternative 1, and is therefore recommended here. Alternative 1 more than likely overestimates the thermal conductivity of this domain, see section 5.4.2.

For domains RSMA and RSMD, results reported for the site descriptive modelling of the Simpevarp subarea version 1.2 /SKB 2005/ are given in Table 5-21 for comparison. It should be noted that in the thermal modelling of domain RSMA in Simpevarp, data from borehole KLX02 in the Laxemar subarea was included, in addition to data from Simpevarp subarea.

Observe that the above table is valid at 20°C. The thermal conductivity decreases slightly at higher temperatures, 1–5°C per 100°C temperature increase.

Table 5-21. Mean thermal conductivity (W/(m·K)) by lithological domain. Comparison with Simpevarp model version 1.2.

Domain	Mean	Mean Simpevarp 1.2.	Comment
RSMA, Ävrö Granite	2.82	2.80[1]	[1]Mean reduced by 0.1 to account for bias in the relationship between density and thermal conductivity for Ävrö granite /Sundberg et al. 2005b/.
RSMBA, Mix of Ävrö granite and fine-grained dioritoid	2.87		
RSMD, Quartz monzodiorite	2.70	2.62[2]	[2]Estimated by Monte Carlo simulation
RSME, Diorite/gabbro	2.45		Estimated by Monte Carlo simulation
RSMM, Mixed zone with large fraction of diorite/gabbro	2.58		Estimated by Monte Carlo simulation

5.5.2 Variability of thermal conductivity

In order to be able to evaluate the spatial variability at domain level, the base approach in addition to the following four complementary approaches have been used as described above:

- Addition of simulated within rock variability from domain RSMA (1).
- Extrapolation of spatial variability (2).
- Subtraction of small scale variability (3).
- Upscaling of "within rock type" variability (4).

The results of each approach are presented in Table 5-22. For the base approach, means and standard deviations are determined for each scale; see Figure 5-12, Figure 5-17 and Figure 5-21. The base approach is believed to underestimate the standard deviation for domain RSMA and RSMBA, but particularly for RSMD, since the within rock variability is not fully accounted for (large difference between domains). As regards domains RSME and RSMM, the base approach overestimates the variability, since no scaling up has been performed.

Table 5-22. Summary of standard deviations (W/(m·K)) at the domain level from modelling results with the base approach compared with the four alternative/complementary approaches (Approaches 1–4). Numbers within brackets are calculated variances, W/(m·K)², with the resulting standard deviations in bold.

Appr.	Scale (m)	RSMA (Ävrö granite)	RSMBA (Mixture of Ävrö granite and Fine-grained dioritoid)	RSMD (Quartz monzodiorite)	RSME (Dioite/ gabbro)	RSMM (mix domain)	Comment
Base	0.8	**0.28** (0.031+0.048 = 0.079) (between rock type + within rock type variance based on 81.5% spatial data)	**0.25** (0.026+0.037 = 0.063) (between rock type + within rock type variance based on 55.5% spatial data)	**0.13** Between rock type variance only (0.016)	**0.29** Monte Carlo sim.	**0.22** Monte Carlo sim.	Underestimation for RSMA RSMBA and RSMD. Overestimation for RSME and RSMM.
1	0.8			**0.25** (0.017+0.048 = 0.065) (between rock type + within rock type variance from RSMA)			Strong overestimation for RSMD.
2	0.8	**0.29** (0.031+0.056 = 0.087) (between rock type +100% within rock type variance)	**0.29** (0.026+0.059 = 0.085) (between rock type +100% within rock type variance)	–	–		Overestimation
3	0.8	**0.30** (0.031+0.062 = 0.093) between rock type variance + (total variance within dominant rock type − small scale variance)	**0.30** (0.026+0.062 = 0.088) between rock type variance + (total variance within rock type − small scale variance from RSMA)	**0.17** (0.017+0.012[1] = 0.029) between rock type variance + (total variance within QMD − small-scale variance)			Overestimation for RSMA and RSMBA. For RSMD, std dev based on the assumption that the effect of upscaling in QMD is equivalent to that for Ävrö granite.
4	0.8	**0.34** (0.031+0.082 = 0.113 (between rock type + within rock type variance)	**0.29** (0.026+0.059[2] = 0.085) (between rock type + within rock type variance)	**0.22** (0.017+0.030[3] = 0.047) (between rock type + within rock type variance at 0.1 m scale)	–		Overestimation for RSMD: effects of upscaling within QMD not considered.

[1] "within rock type" variance at 0.8 m scale for quartz monzodiorite (QMD) calculated by assuming that small-scale variance, i.e. 0–0.8 m, accounts for 37% of the total variance.

[2] Approximation of internal spatial variance within the rock types in the domain assuming a composition of 64% Ävrö granite and 36% fine-grained dioritoid (0.64·0.082+0.36·0.018 = 0.059), see Table 5-4.

[3] Approximation of internal spatial variance within the rock types in the domain calculated assuming a composition of 84% quartz monzodiorite and 16% Ävrö granite (0.84·0.020+0.16·0.082 = 0.030).

Approach 1 almost certainly overestimates spatial variability for RSMD since the dominant rock type in this domain, quartz monzodiorite, is considered to display less “within rock type” variation than does Ävrö granite. The latter displays an unusually wide compositional variation /Wahlgren et al. 2005b/, a fact reflected in the large range of measured and calculated thermal conductivity values, see Table 4-22. As described in previous sections, approach 2 most likely overestimates the standard deviation. Theoretically, approach 3 should overestimate the standard deviation, since the variance within the dominant rock type, i.e. Ävrö granite, is considered to represent the domain as a whole. It is not easy, generally speaking, to assess whether Approach 4 under- or overestimates the total variance for a domain. For domain RSMBA, which comprises two dominant rock types, the total within rock type variance is approximated by summing the two “within rock type” variances weighted according to their abundance in the domain. For domain RSMD, however, an upper limit for the standard deviation at the 0.8 m scale is provided by Approach 4, since variance reduction due to upscaling within quartz monzodiorite, the dominant rock type, was not considered. The resulting standard deviation (0.22 W/(m·K)) is essentially the same as the standard deviation produced by the base approach for the 0.1 m scale (Table 5-11), a scale at which all within rock variability should be included.

Taking into account the outcomes of the different approaches, the following standard deviations for each domain are proposed.

- Both domain RSMA and RSMBA are attributed the concluding value of 0.29 W/(m·K), which is the result from approach 2 at the 0.8 m scale.
- For domain RSMD, the standard deviation given by Approach 3, 0.17 W/(m·K), is adopted. Since a variance reduction due to upscaling is to be expected, this approach is considered to provide a more reasonable approximation of spatial variability for this domain.
- For domains RSME (diorite/gabbro) and RSMM (mixed zone with large fraction of diorite/gabbro), no changes have been made in the standard deviation compared with the simulation results of the base approach.

Table 5-23 summarises the mean and revised standard deviation for each domain.

Observe that the above table is valid at 20°C. The thermal conductivity decreases slightly at higher temperatures, 1–5°C per 100°C temperature increase.

Table 5-23. Mean and revised standard deviation of thermal conductivity (W/(m·K)) per domain at the 0.8 m scale. Differences between revised and modelled (base approach) standard deviation are quoted for domains RSMA, RSMBA and RSMD. For RSME and RSMM results are based on distributions derived from realisations from Monte Carlo simulation.

Domain	Mean	Std dev	Diff	Comment
RSMA	2.82	0.29	+0.014	Approach 2
RSMBA	2.87	0.29	+0.040	Approach 2
RSMD	2.70	0.17	+0.043	Approach 3
RSME	2.45	0.29		No changes in std dev from MC simulation
RSMM	2.58	0.22		No changes in std dev from MC simulation

5.5.3 Estimation of lower tail percentiles of thermal conductivity

Since the distributions of thermal conductivities at domain level cannot be shown to be normal, estimations of lower and upper tail percentiles based on the revised standard deviations cannot be calculated using parametric methods. To estimate lower and upper tail percentiles for the revised standard deviations, corrections were made to the percentile values calculated from the modelled distributions (Table 5-24). As already mentioned, the lower tail percentiles are of most interest as it is these that are critical for design purposes.

For each domain, the correction involved the following steps:

1. The 0.5, 2.5 and 97.5 percentiles were estimated from the modelled data distributions using the base approach (A in Table 5-24).
2. The 0.5, 2.5 and 97.5 percentiles were estimated using both the modelled standard deviations (Table 5-14) and revised standard deviations (Table 5-23), this time assuming a normal distribution. The difference between these two estimates was determined for each percentile (B in Table 5-24).
3. The differences in step 2 are, as appropriate, subtracted from or added to the percentile values given by the base approach distributions in step 1.

The resulting values are suggested to be reasonable approximations of the respective percentiles for the 0.8 m scale. It should be mentioned that uncertainties associated with estimation of percentiles become larger at the more extreme ends of the distributions. As an additional check on the reasonableness of these suggested values, the percentiles based on the modelled results in the base approach at the 0.1 m scale are presented (Table 5-24). These provide a theoretical lower limit for the lower tail percentiles at larger scales. The approximated percentiles at scale 0.8 m are, not surprisingly, significantly higher than those for the 0.1 m scale estimated from modelling results.

Table 5-24. Approximations of 0.5, 2.5 and 97.5 percentiles of thermal conductivity (W/(m·K)) for domains RSMA, RSMBA and RSMD at the scale 0.8 m.

Domain	From modelled data distribution, Table 5-14 (A)	Diff according to revised std dev assuming normal distribution (B)	Approximated value: for lower tail percentiles (A–B); for upper tail percentiles (A+B)	0.1 m scale from base approach
	0.5 percentiles			
RSMA	2.24	0.04	2.20	2.01
RSMBA	2.34	0.10	2.24	1.95
RSMD	2.43	0.11	2.32	2.13
	2.5 percentiles			
RSMA	2.35	0.03	2.32	2.22
RSMBA	2.45	0.08	2.37	2.16
RSMD	2.52	0.08	2.44	2.35
	97.5 percentiles			
RSMA	3.37	0.03	3.39	3.54
RSMBA	3.35	0.08	3.43	3.60
RSMD	3.10	0.08	3.19	3.32

Because no scaling up has been performed for domains RSME and RSMM, the quoted lower tails estimated from realisations based on Monte Carlo simulation are conservatively low for larger scales. By taking into account the effect of upscaling on lower and upper tail percentiles observed in the other domains, which on average is about 0.2 W/(m·K) for the 0.8 m scale, corrected 0.5, 2.5 and 97.5 percentiles can be approximated for domains RSME and RSMM, see Table 5-25. Obviously, these approximations are very uncertain.

Observe that the above table is valid at 20°C. The thermal conductivity decreases slightly at higher temperatures, 1–5% per 100°C temperature increase.

Table 5-25. Rough approximations of 0.5, 2.5 and 97.5 percentiles of thermal conductivity (W/(m·K)) for domains RSME and RSMM at the scale 0.8 m.

	0.5 percentiles		2.5 percentiles		97.5 percentiles	
Domain	From base approach: 0.1 m scale	Approximation after correction for upscaling	From base approach: 0.1 m scale	Approximation after correction for upscaling	From base approach: 0.1 m scale	Approximation after correction for upscaling
RSME	1.85	2.0	1.98	2.2	3.22	3.0
RSMM	1.98	2.2	2.13	2.3	2.98	2.8

5.5.4 Comparsion with previous model versions

A comparison of the thermal conductivity results for domain level presented in the site descriptive model Simpevarp version 1.1 /SKB 2004/, site descriptive model Simpevarp version 1.2 /SKB 2005/, and the current Laxemar 1.2 site descriptive model version is provided in Table 5-26. The differences in mean and standard deviation of thermal conductivity for domain RSMA between Simpevarp 1.2 and Laxemar 1.2 are small. For domain RSMD the mean is somewhat higher in Laxemar 1.2, whereas the standard deviation is much lower.

Observe that the above table is valid at 20°C. The thermal conductivity decreases slightly at higher temperatures, 1–5% per 100°C temperature increase.

Table 5-26. Comparison of modelling results (the mean and the standard deviation) from Simpevarp 1.1, Simpevarp 1.2 and Laxemar 1.2 site descriptive model versions.

	Mean (W/(m·K))				Std dev (W/(m·K))		
Domain	Version S1.1	Version S1.2	Version L1.2	Diff (L1.2–S1.2)/ S1.2	Version S1.1	Version S1.2	Version L1.2
RSMA	2.67	2.80	2.82	0.7%	0.25	0.28	0.29
RSMD	2.38	2.62	2.70	3.1%	0.10	0.28	0.17

5.5.5 Discussion

The method used above to approximate percentiles is associated with uncertainties. More refined modelling strategies are required to describe the spatial variability of thermal properties at domain level more satisfactorily. One way is to generate representative statistical distributions of thermal conductivity, perhaps using a variety of approaches, in which both “between rock type” and “within rock type” variabilities are considered. From these realisations, means, standard deviations and any desired percentile can be estimated. A proposed project dealing with modelling strategies aims to resolve these issues.

The high noise in the density logging data, on which much of the modelling relies, is an important source of uncertainty impacting on the results. In particular, the considerable random noise in the logging data is producing thermal conductivity values at the 0.1 m scale which are unreasonably low (1.84 W/(m·K)). Such low conducting rocks are highly improbable in Laxemar (see below). Fortunately, an “evening-out” effect occurs as a result of upscaling, so that at 0.8 m scale the minimum value rises to 2.10 W/(m·K). If the density relationship was not extrapolated to thermal conductivities below say 2.2 W/(m·K), but was instead restricted to a narrower interval, then a serious bias would be generated in our modelling results, the magnitude of which would be difficult to assess. With considerable justification, therefore, the latter approach was rejected.

One objective of the modelling work reported here has been to quote lower limits of thermal conductivity distributions in different domains, at a scale that is relevant for the canister in a deep repository. The 0.5 and 2.5 percentiles quoted in Table 5-24 and Table 5-25 are the results of our attempts to achieve this based on the available data, which it must be underlined has limitations concerning degree of representativeness as well as other uncertainties. In other words, new and more representative data may produce somewhat different results. It should also be noted that the quoted lower tail percentiles are based on the results of the modelled distributions, and no confidence intervals for these percentiles have been estimated. Precision in the estimation of percentiles in the extreme tails of a distribution is obviously lower than for less extreme percentiles.

The recommended approximations of lower tail percentiles may be underestimating the true values (conservatively low) at a scale that is relevant for the canister. One reason for this is that the scale chosen (0.8 m) to present the results may be somewhat conservative. Work at the Äspö HRL indicates that variability at scales below between 1 and 2 m are irrelevant for the temperature at the canister /Sundberg et al. 2005a/. Upscaling to 2 m would result in 0.5 and 2.5 percentiles about 0.1 W/(m·K) higher than those given by the 0.8 m scale, based on results indicated by the base approach. On the other hand, recent results, not reported here, indicate that, for low thermal conductivity Ävrö granite, conductivity values from density logging may be overestimated by as much as 0.1 W/(m·K). If it is assumed that these effects tend to cancel each other out, then it can be argued that the recommended approximations of lower tail percentiles are quite reasonable.

At the present state of knowledge, it is difficult to accurately quote a minimum value of thermal conductivity for the different domains. Of the common rock-forming minerals, plagioclase has the lowest thermal conductivity. A theoretical absolute minimum of about 1.6 W/(m·K) for crystalline rocks is provided by a hypothetical igneous rock consisting of 100% plagioclase. The closest one comes to rocks with such compositions are anorthosites, which per definition are intrusive igneous rocks consisting of more than 90% plagioclase. Such rocks have not been reported from the investigated area. Rocks comprising up to 63% plagioclase have been recorded in the Laxemar/Simpevarp area. The lowest thermal conductivity measured in the laboratory for all rock types is 2.16 W/(m·K), for a sample of Ävrö granite from Äspö. Recent measurements on Ävrö granite samples from the Laxemar subarea, which were not included in the data freeze for Laxemar 1.2, indicate even lower thermal conductivities. So, in the light of these results, the lower 0.5 percentile value of 2.20 W/(m·K) recommended here for domain RSMA is not unreasonable.

Both geological mapping and modal analysis of thin sections have shown that there is considerable compositional variation within the Ävrö granite /SKB 2006/. Not surprisingly, this is reflected in the wide spread of thermal conductivity values within this rock type, both measured on core samples and modelled from modal analyses and density loggings. Thermal conductivity calculations based on mineral composition (SCA data) from surface samples indicate a central area of Ävrö granite characterised by high thermal conductivities flanked by areas to the north and south with lower values. A similar picture emerges with depth in the few boreholes that have been investigated. Ävrö granite with low thermal conductivities is mainly found in borehole KLX03 to the south and KLX01 to the north, while Ävrö granite with relatively high conductivities occurs in the centrally located boreholes, namely KLX02 and KLX04. This unambiguous geographical heterogeneity within the Ävrö granite requires additional study in order to acquire a 3D understanding of the spatial variability of thermal properties within the RSMA domain.

Uncertainties associated with the determination of the mean thermal conductivity for domain RSMM are particularly great. Firstly, there is an incomplete understanding of the proportions of different rock types that comprise this domain. Secondly, recent TPS measurements of diorite/gabbro samples indicate that variability in thermal conductivity for this rock type is greater than that specified by the rock type model used in this study. Finally, in the absence of density logging data, there are uncertainties resulting from the choice of rock type model for Ävrö granite.

In this report, the modelling results for domain RSMBA are based on data from RSMBA03, one of three identified BA subdomains in Laxemar. The other two, RSMBA01 and RSMBA02, occur in south Laxemar and, at least at the surface, are enclosed within domain RSMM01. Although the general lithological makeup of all three appears similar, no definite conclusions regarding the thermal properties of the two southern occurrences can be made. Given the established quartz-poor and low conductive nature of the Ävrö granite in south Laxemar, it is plausible that both RSMBA01 and RSMBA02 have lower mean thermal conductivities than RSMBA03.

5.6 Summary of domain properties

5.6.1 Thermal conductivity

Table 5-27 summarises the recommended mean, standard deviation and lower bounds of thermal conductivity for each domain. Observe that these results are valid at 20°C. The thermal conductivity decreases slightly at higher temperatures, by 1–5% per 100°C temperature increase.

Table 5-27. Recommended mean, standard deviation and lower tail percentiles of thermal conductivity (W/(m·K)) per domain at 0.8 m scale. For RSME and RSMM, a rough correction has been applied to percentiles estimated from Monte Carlo simulated distributions, which are based on a < 0.1 m scale.

Domain	Mean	Std dev	0.5 percentile	2.5 percentile
RSMA	2.82	0.29	2.20	2.32
RSMBA	2.87	0.29	2.24	2.37
RSMD	2.70	0.17	2.32	2.44
RSME	2.45		2.0	2.2
RSMM	2.58		2.2	2.3

5.6.2 Heat capacity

Modelling of heat capacity on domain level is performed as a Monte Carlo simulation where the occurrence of different rock types in the domain is weighted together with the rock type models. Results presented in Table 5-20 for four domains indicate a small range (2.23–2.29 MJ/(m·K)) in mean heat capacity. Observe that these results are valid at 20°C. The heat capacity increases by approximately 25% per 100°C for the dominating rock types.

5.6.3 Coefficient of thermal expansion

No domain modelling has been made. It is suggested that the mean value for the dominant rock in each domain in Table 4-25 is representative for the whole domain.

5.6.4 In situ temperature

Domain modelling has not been performed. For all domains, a mean of the in situ temperature at 400, 500 and 600 m depth is estimated at 12.3, 13.9 and 15.6°C, respectively, see Section 4.11.2.

6 Evaluation of uncertainties

A general description of uncertainties is provided in the strategy report for the thermal site descriptive modelling /Sundberg, 2003a/. In /Sundberg et al. 2005a/ a conceptual uncertainty model is presented. Uncertainties are introduced at the following levels/stages:

- Data level.
- Rock type level.
- Domain level.

Qualitative estimates of the various types of uncertainties are given in, Table 6-1, Table 6-2 and Table 6-3 for the three different levels. However, only a number of them are believed to significantly affect the results at canister scale. Of major interest is the total uncertainty in thermal conductivity at the canister scale at domain level, since this affects the design of the repository.

6.1 Thermal conductivity

6.1.1 Data level

Uncertainty at the data level results in data with a random or systematic deviation from the correct value for a sample. This applies to thermal conductivity data from TPS measurements, calculations with the SCA method, and calculations based on density measurements. Table 6-1 summarises these uncertainties.

TPS data

The accuracy of TPS measurements is better than 5% and the repeatability is better than 2% according to the manufacturer of the measurement equipment /Sundberg 2002/. The mean difference in the results of thermal conductivity measurements on the same samples performed by different laboratories using the same method is less than 2%.

Note that this uncertainty refers to the measurement volume (approx. 10 cm^3) and not the volume of the sample, since only a subvolume of the sample is subject to measurement. If the TPS measurement is assumed to represent the sample scale (approx. 100 cm^3) the uncertainty is larger, an effect of the small-scale heterogeneity of the rock.

There is a potential bias (underestimation) in thermal conductivity data. The reason is that stress dependence has not been assessed. Measurements are made on stress released samples. However, the effect is assumed to be low since the samples are water saturated before measurement.

Table 6-1. Uncertainty in thermal conductivity data at data level. Each uncertainty consists of a random and a systematic part. Subjective qualitative estimates are given in three classes; small, medium and large uncertainty.

Uncertainty in:	Random uncertainty (expected random variation)	Systematic uncertainty (expected bias)
TPS data		
Measurement technique	small	small
Measurement scale vs sample	medium	small
SCA data		
Determination volume fraction of minerals	small	medium
Alteration of minerals	medium	large
Thermal conductivity of minerals	–	medium
Method for calculation of thermal conductivity	small	small
Modal analysis scale vs sample	large	small
Density logging data		
Measurement technique, including filtering and recalibration	large	small
Measurement scale	small	small
Statistical relationship between thermal conductivity and density, including scale representativeness, laboratory density measurements, rock type classification, natural variability, and selection of regression model	large	medium
All data		
Database errors (SICADA. Remaining after quality control)	small	small

SCA data

The uncertainty associated with SCA data is significantly larger than for TPS data. For SCA data one of the most important sources of uncertainty is caused by alteration of minerals. An example of this type of uncertainty is that some minerals, typically plagioclase and biotite, have been subjected to partial alteration, to sericite and chlorite respectively. In most cases quantitative analysis of the extent of alteration has not been performed. The lack of consideration of the presence of alteration products almost certainly leads to bias, since the thermal conductivities of these alteration minerals differs from those of the parent mineral. For rock types where a comparison of SCA and TPS data for the same samples is possible, a correction factor has been applied to the SCA data. Another uncertainty relates to the values of thermal conductivity assigned to the different minerals. Derived from literature, these thermal conductivity values may vary considerably depending on the composition of the mineral in the actual sample, especially for plagioclase, pyroxene, and olivine.

Density data

Thermal conductivities are calculated for Ävrö granite based on density loggings using the relationship in Figure 4-13. It is believed that uncertainties associated with the density loggings dominate for domains where Ävrö granite is of importance. The major uncertainties associated with this procedure are:

- the high noise level in the density logging data (measurements),
- the statistical relationship between density and thermal conductivity.

Potential random errors due to noise might, for some of the boreholes, be as high as 50–60 kg/m^3 /Mattsson and Thunehed 2004, Mattsson 2004a/. The noise in density loggings can be reduced by improving the density logging technique. The statistical relationship between density and thermal conductivity can be improved by performing a large number of measurements (density and thermal conductivity) on rock samples of Ävrö granite in the Laxemar subarea. There is also potential bias in the values calculated from density measurement. This would be the case if the observed density vs thermal conductivity relationship did not accurately represent the rock volume in the Laxemar subarea.

Natural variability of mineral composition within Ävrö granite results in variability of both density and thermal conductivity, but the regression equation is only an approximation and is not capable of capturing all this variability.

6.1.2 Rock type level

Uncertainty at the rock type level results in thermal conductivity estimates (PDF, mean and variance) that deviate from the true distribution for the rock type. Causes of uncertainty are presented in Table 6-2. Important causes are the issue of representativeness and the selection of rock type models.

Representativeness of data

The representativeness of samples selected for TPS measurements is less than satisfactory. The samples are not taken with the purpose of statistically representing the rock mass, and consequently there is a potential for bias. As an example, TPS samples from both the Laxemar and Simpevarp subareas are often taken in groups of up to 5 samples from a limited section of the borehole (1 or 2 m). As regards the calculated values based on modal analyses (SCA method) representativeness is considerably better for the major rock types, since sampling has been carried out at a greater number of locations. For subordinate rock types, representativity and low number of samples contribute to uncertainty.

As evidence by the boremap mapping of the Laxemar boreholes /SKB 2006/, a significant volume, 10–15%, is comprised of weakly to strongly altered rocks. These altered rocks have not been sampled for measurement of thermal properties. This may have introduced a bias to the results.

Table 6-2. Uncertainty in thermal conductivity data at rock type level. Each uncertainty consists of a random and a systematic part. Subjective qualitative estimates are given in three classes; small, medium, and large uncertainty.

Uncertainty in:	Random uncertainty (expected random variation)	Systematic uncertainty (expected bias)
All thermal data		
Boremap logging and classification of rock samples	small	small – medium
Temperature and pressure effects	small	small
Representativeness of data	–	large
Method of correction, SCA data	–	medium
Spatial variability within rock type	natural (large)	–
Statistical model, PDF (assumptions)	small	small

Rock type models

For fine-grained dioritoid and quartz monzodiorite the rock type models are based on TPS data and corrected SCA data. The correction is based on comparison of SCA data with TPS data. Because the comparison is based on only a few samples, there is uncertainty in the accuracy of this correction. For the other rock type models, no correction was performed due to lack of data, which of course leads to uncertain models.

Normal distribution models (PDF:s) were chosen to characterize the rock types. There is a slight deviation between data and model. Generally, the rock type models slightly overestimate the occurrence of small thermal conductivity values and underestimate the number of large values.

The data set is very small for several rock types, which implies that these rock type models are highly uncertain. This applies to fine-grained diorite-gabbro (505102), diorite/gabbro (511033), granite (501058), and fine-grained granite (511058).

Spatial variability within rock type

A model of spatial variability within rock type has only been developed for Ävrö granite, see section 4.7. It is primarily based on density logging data, with its inherent noise and potential bias. For other rock types, spatial variability is only considered in the alternative approaches of domain modelling.

6.1.3 Domain level

Uncertainty at the domain level results in thermal conductivity estimates (mean, standard deviation and percentiles) that deviate from the true distribution of values at the scale of interest. Sources of uncertainty are given in Table 6-3. The most important are the geological model, the related issue of representativeness of boreholes, the choice of significant scale for the canister, the upscaling methodology in the modelling, and spatial variability both within and between rock types. In addition, there are also a number of other uncertainties of less importance.

Geological model

It is not known how large the uncertainties in the geological model are.

Deformation zones

Influences from fractures and deformation zones on thermal properties have not been considered. No thermal data is available from the deformation zones. Neither has the thermal influence of water movements been considered in the modelling. However, it is not envisaged that fracture zones will be present near the deposited canisters.

Representativeness of boreholes

The representativeness of the boreholes is believed to be the most important uncertainty of all. Boreholes that do not represent the rock mass of interest will lead to biased results, and highly unrepresentative boreholes may give false indications of the thermal properties. A highly sophisticated modelling cannot combat this. Comparison of different boreholes may give indications if there is a potential for large bias due to bad representativeness.

Table 6-3. Uncertainty in thermal conductivity data at domain level. Each uncertainty consists of a random and a systematic part. Subjective qualitative estimates are given in three classes; small, medium, and large uncertainty.

Uncertainty in:	Random uncertainty (expected random variation)	Systematic uncertainty (expected bias)
Canister scale		
Geological model (boremap logging, rock type occurrence, extension of domains)	large	–
Deformation zones, fractures etc	medium	medium
Water flow	small	large
Core logging: boremap	–	small
Representativeness of boreholes	–	large
Estimated proportions of rock types	–	large
Spatial variability within domain	natural (large)	–
Anisotropy	small	small
Upscaling methodology	medium	small
Significant scale for the canister	small	medium
Statistical model (assumptions of distribution, percentile estimation etc)	small	small

This is certainly the case for domain RSMA, which is dominated by Ävrö granite, a rock type with large spatial variability. Uncertainty can be reduced by increasing the number of boreholes. In this regard the modelling results presented here for domain RSMA represent an improvement on models developed for Simpevarp versions 1.1 and 1.2. Domain RSMD, dominated by quartz monzodiorite, would appear to have less inherent variability.

The random part of the uncertainty can be estimated by careful comparison of data from different boreholes.

Estimated proportions of rock types

Estimations of the proportion of rock types in domains not modelled using borehole data, namely RSME and RSMM, are associated with uncertainties. These uncertainties have not been accommodated in the modelling of thermal properties.

Spatial variability within the domain

Spatial variability within the domain is handled by modelling, see section 5.3. This is a non-reducible uncertainty, only the uncertainty about the true state of variability can be reduced.

Upscaling methodology

For all rock types except Ävrö granite, thermal conductivity values are randomly assigned at the 0.1 m scale based on the rock type models. These rock type models probably overestimate the variance at the 0.1 m scale. The reason is that TPS and SCA data represent a smaller scale. At the 0.1 m scale, some reduction of variance should already have taken place. Therefore, this approach overestimates the likelihood of small values.

In the base modelling approach, spatial variability within rock types other than Ävrö granite is ignored. This results in too large a variance reduction when the scale increases. To compensate for this, complementary approaches have been employed to take into account the variance due to spatial variability within other rock types. These approaches involve some uncertainties. These include the procedure used in approach 2 for adjustment of spatial variability, the addition and subtraction of variances in approaches 1–4, and the estimation of spatial variability from variograms (approach 3) and TPS data (approach 4). These uncertainties all arises from lack of knowledge of spatial variability within the rock types and within the domains. The most straight-forward way of reducing this uncertainty is to collect considerably more data. Apart from the need for more data, one way of overcoming this problem is to produce data sets by stochastic simulation that contains both variability within rock types and variability between rock types. This will eliminate the need for further adjustment of variances and percentiles, as described in section 5.5.2.

Anisotropy

Measurements to assess the anisotropy in thermal conductivity and thermal diffusivity have not been carried out as part of the current data freeze. Large-scale anisotropy produced by the preferential orientation of subordinate rock types should also be evaluated.

Significant scale for the canister

Another source of uncertainty in the thermal modelling is the scale at which thermal conductivity is significant for the heat emitted from the canister. To reduce this uncertainty numerical simulation of heat flow has been performed /Sundberg et al. 2005a/. Results indicate that variations in thermal conductivity at scales lower than 1–2 m are irrelevant for the temperature on the canister. Therefore, modelling approaches in this report have focused mainly on the 0.8 m scale, a sufficiently small scale so as not to underestimate the variability. However, no measurements of thermal properties at these scales have been conducted to confirm the results.

Statistical model

The recommended lower tail percentiles of thermal conductivity (0.5 and 2.5 percentiles) for each domain are partly based on differences observed between distributions that are assumed to be normally distributed. The performed adjustment of the percentiles is evidently associated with uncertainty. The percentiles are also uncertain due to the limited amount of data in the low tails of the data distributions. For domain RSMA, 95% confidence intervals of the 0.5 and 2.5 percentiles have been estimated by a nonparametric method, according to /Mac Berthouex and Brown 2002/. The result indicates an uncertainty of approximately ± 0.05 W/(m·K) for the 0.5 percentile and ± 0.02 W/(m·K) for the 2.5 percentile. This uncertainty is believed to be lower than the uncertainties associated with the estimation of percentiles.

Several stages in the modelling are based on addition of variances due to variability within rock types and variability between rock types. It should be noted that this methodology only produces rough estimates of the total variance. Addition and subtraction of variances will result in over- or underestimation depending on the assumptions made for the particular domain and approach. One way of overcoming this problem is to produce data sets by stochastic simulation that contains both variability within rock types and variability between rock types. This will eliminate the need for further adjustment of variances and percentiles, as described in the later stages of this report.

6.2 Heat capacity

A problem exists with the representativeness of measured values (TPS data). Samples are in several cases focused to certain limited parts of the rock mass. For quartz monzodiorite the number of samples is rather small.

Subordinate rock types have not been considered when modelling the heat capacity.

The modelling is based on TPS data which means a scale less than 0.1 m. Since mean values and standard deviations show only a small variation between rock types, and since the data is normally distributed, the properties in larger scales can be expected to be basically the same.

No direct laboratory measurements of heat capacity have been performed. Instead, heat capacity has been determined through conductivity and diffusivity measurements performed with the TPS method.

6.3 In situ temperature

Temperature loggings from different boreholes show large variations in temperature at a specific depth. Borehole KLX01, for example, displays significantly higher temperatures than other boreholes. The difference implies an uncertainty in temperature loggings and even small uncertainties may influence the design.

There is an uncertainty in the results from the temperature loggings. Errors associated with calibration of the temperature sensors have recently been recognized, so that accuracy is no better than ± 2°C. The equipment is now reconstructed, and future measurements will have accuracy better than ± 1°C.

Other possible sources of uncertainty are timing of the logging after drilling (drilling adds to temperature disturbance), water movements along the boreholes and uncertainty in the measured inclination of the boreholes. The uncertainty imposed by water movements can be evaluated jointly with the hydrogeologists. However, this has not yet been done.

6.4 Thermal expansion

There is a problem with the representativeness of the measurements, due to the availability of only a small number of samples concentrated to certain parts of the rock volume.

Pressure dependence on thermal expansion has not been investigated but may have a significant influence on the results.

References

Adl-Zarrabi B, 2004a. Drill hole KSH01A: Thermal properties: heat conductivity and heat capacity determined using the TPS method and mineralogical composition by modal analysis. SKB P-04-53, Svensk Kärnbränslehantering AB.

Adl-Zarrabi B, 2004b. Drill hole KSH02: Thermal properties: heat conductivity and heat capacity determined using the TPS method and mineralogical composition by modal analysis. SKB P-04-54, Svensk Kärnbränslehantering AB.

Adl-Zarrabi B, 2004c. Drill hole KAV01: Thermal properties: heat conductivity and heat capacity determined using the TPS method and mineralogical composition by modal analysis. SKB P-04-55, Svensk Kärnbränslehantering AB.

Adl-Zarrabi B, 2004d. Drill hole KAV04A: Thermal properties: heat conductivity and heat capacity determined using the TPS method and mineralogical composition by modal analysis. SKB P-04-270, Svensk Kärnbränslehantering AB.

Adl-Zarrabi B, 2004e. Drill hole KLX02: Thermal properties: heat conductivity and heat capacity determined using the TPS method and mineralogical composition by modal analysis. SKB P-04-258, Svensk Kärnbränslehantering AB.

Adl-Zarrabi B, 2004f. Drill hole KLX04: Thermal properties: heat conductivity and heat capacity determined using the TPS method and mineralogical composition by modal analysis. SKB P-04-267, Svensk Kärnbränslehantering AB.

Dagan, 1979. Models of groundwater flow in statistically homogenous porous formations. Water resources res., 15 (1), 47–63.

Dinges C, 2004. Drill hole KSH01A. Thermal properties: thermal conductivity and specific heat capacity determined using the Hot Disk thermal constants analyser (the TPS technique) – Compared test. SKB P-04-160, Svensk Kärnbränslehantering AB.

Goovaerts P, 1999. Geostatistics in soil science: state-of-the-art and perspectives. Geoderma, 89 (1999): 1–45.

Gilbert R, 1987. Statistical methods for Environmental Monitoring, New York, Van Nostrand Reinhold.

Gustafsson S, 1991. Transient plane source techniques for thermal conductivity and thermal diffusivity measurements of solid materials. Rev. Sci. Instrum. 62, p 797–804. American Institute of Physics, USA.

Gutjahr A L, Gelhar L W, Bakr A A, MacMillan J R, 1978. Stochastic analysis of spatial variability in subsurface flows. 2. Evaluation and application. Wat. resorces res., vol. 14, no 5. p 953–959.

Hashin Z, Shtrikman S, 1962. A variational approach to the theory of the effective magnetic permeability of multiphase materials, J. Appl. Phys. 33, 3125.

Horai K, 1971. Thermal conductivity of rock-forming minerals. J. Geophys. Res. 76, p 1,278–1,308.

Horai K, Baldridge S, 1972. Thermal conductivity of nineteen igneous rocks, Application of the needle probe method to the measurement of the thermal conductivity of rock. Estimation of the thermal conductivity of rock from the mineral and chemical compositions. Phys. Earth Planet. Interiors 5, p 151.

HotDisk, 2004. www.hotdisk.se, access 2004-09-22.

Isaaks E H, Srivastava R M, 1989. An introduction to applied geostatistics. Oxford University Press, New York.

Mac Berthouex P, Brown L C, 2002. Statistics for environmental engineers, 2nd edition. Lewis Publishers.

Mattsson H, 2004a. Interpretation of geophysical borehole data and compilation of petrophysical data from KSH03A (100–1,000 m), KSH03B, HAV09, HAV10 and KLX02 (200–1,000 m). Oskarshamn site investigation. SKB P-04-214, Svensk Kärnbränslehantering AB.

Mattsson H, 2004b. Interpretation of geophysical borehole data and compilation of petrophysical data from KAV04A (100–1 000 m), KAV04B, HLX13 and HLX15. Oskarshamn site investigation. SKB P-04-217, Svensk Kärnbränslehantering AB.

Mattsson H, Thunehed H, 2004. Interpretation of geophysical borehole data and compilation of petrophysical data from KSH02 (80–1,000 m) and KAV01. SKB P-04-77, Svensk Kärnbränslehantering AB.

Mattsson H, Thunehed H, Triumf C A, 2004. Compilation of petrophysical data from rock samples and in-situ gamma-ray spectrometry measurements. Oskarshamn site investigation. SKB P-04-294, Svensk Kärnbränslehantering AB.

Mattsson H, 2005. GeoVista AB, Personal communication.

Mattsson H, Thunehed H, Keisu, M, 2005. Interpretation of geophysical borehole measurements and compilation of petrophysical data from KLX01, KLX03, KLX04, HLX21, HLX22, HLX23, HLX24, HLX25, HLX26, HLX27 and HLX28. Oskarshamn site investigation. SKB P-05-34, Svensk Kärnbränslehantering AB.

Nilsson K P, Bergman T, Eliasson T, 2004. Bedrock mapping 2004 – Laxemar subarea and regional model area. Outcrop data and description of rock types. Oskarshamn site investigation. SKB P-04-221, Svensk Kärnbränslehantering AB.

Nielsen T, Ringgaard J, Horn F, 2004. Geophysical borehole logging in boreholes KSH02 and KLX02. SKB P-03-111, Svensk Kärnbränslehantering AB.

Nielsen T, Ringgaard J, 2004. Geophysical borehole logging in boreholes KAV04A, KAV04B, HLX13 and HLX15. SKB P-04-202, Svensk Kärnbränslehantering AB.

Nielsen T, Horn F, 2004. Geophysical borehole logging in boreholes KLX03, HLX21, HLX22, HLX23, HLX24 and HLX25. SKB P-04-280, Svensk Kärnbränslehantering AB.

Nielsen T, Ringgaard J, Horn F, 2004. Geophysical borehole logging in boreholes KLX04, HLX26, HLX27 and HLX28. SKB P-04-306, Svensk Kärnbränslehantering AB.

Rouhiainen P, Pöllänen J, Sokolnicki, 2005. Oskarshamn site investigation, Difference flow logging of borehole KLX03, Subarea Laxemar. SKB P-05-67, Svensk Kärnbränslehantering AB.

Sandström M, 2005. Boreholes KFM01A and KSH01A: Inter-laboratory comparison of rock mechanics testing results. SKB P-05-239, Svensk Kärnbränslehantering AB.

SKB, 2004. Preliminary Site Description, Simpevarp area – version 1.1. SKB R-04-25, Svensk Kärnbränslehantering AB.

SKB, 2005. Preliminary Site Description, Simpevarp subarea – version 1.2. SKB R-05-08, Svensk Kärnbränslehantering AB.

SKB, 2006. Preliminary Site Description Laxemar subarea – version 1.2. Svensk Kärnbränslehantering AB. Report in progress.

Sundberg J, 1988. Thermal properties of soils and rocks, Publ. A 57 Dissertation. Department of Geology, Chalmers University of Technology and University of Göteborg, Sweden.

Sundberg J, Gabrielsson A, 1999. Laboratory and field measurements of thermal properties of the rock in the prototype repository at Äspö HRL. SKB IPR-99-17, Svensk Kärnbränslehantering AB.

Sundberg J, 2002. Determination of thermal properties at Äspö HRL. Comparison and evaluation of methods and methodologies for borehole KA 2599 G01. SKB R-02-27, Svensk Kärnbränslehantering AB.

Sundberg J, 2003a. A strategy for the model development during site investigations version 1.0. SKB R-03-10, Svensk Kärnbränslehantering AB.

Sundberg J, 2003b. Thermal properties at Äspö HRL. Analysis of distribution and scale factors. SKB R-03-17, Svensk Kärnbränslehantering AB.

Sundberg J, Back P-E, Hellström G, 2005a. Scale Dependence and Estimation of Rock Thermal Conductivity. Analysis of Upscaling, Inverse Thermal Modelling and Value of Information with the Äspö HRL Prototype Repository as an Example. SKB R-05-82, Svensk Kärnbränslehantering AB.

Sundberg, J, Back, P-E, Bengtsson, A, Ländell, M, 2005b. Oskarshamn site investigation. Thermal modelling of the Simpevarp Area – Supporting document for thermal model version 1.2. SKB R-05-24, Geo Innova AB, Svensk Kärnbränslehantering AB, Stockholm.

Triumf C-A, Thunehed H, Kero L, Persson L, 2003. Oskarshamn site investigation. Interpretation of airborne geophysical survey data . Helicopter borne survey data of gamma-ray spectrometry, magnetics and EM from 2002 and fixed-wing airborne survey of data of the VLF-filed from 1986. SKB P-03-100, Svensk Kärnbränslehantering AB.

Wahlgren C-H, 2004. SGU **(**Geological Survey of Sweden); personal communication.

Wahlgren C-H, Ahl M, Sandahl K-A, Berglund J, Petersson J, Ekström M, Persson P-O, 2004. Bedrock mapping 2003 – Simpevarp subarea. Outcrop data, fracture data, modal and geochemical classification of rock types, bedrock map, radiometric dating. SKB P-04-102, Svensk Kärnbränslehantering AB.

Wahlgren C-H, Hermanson J, Curtis P, Forssberg O, Triumf C-A, Tullborg E-L, Drake H, 2005a. Geological description of rock domains and deformation zones in the Simpevarp and Laxemar subareas. Preliminary site description, Laxemar subarea, version 1.2. SKB R-05-69, Svensk Kärnbränslehantering AB.

Wahlgren C-H, Bergman T, Nilsson K, Eliasson T, Ahl, M, Ekström M, 2005b. Bedrock map of the Laxemar subarea and surroundings. SKB R-05-180, Svensk Kärnbränslehantering AB.

Åkesson U, 2004a. Drill hole KSH01A Extensometer measurements of the coefficient of thermal expansion of rock. SKB P-04-59, Svensk Kärnbränslehantering AB.

Åkesson U, 2004b. Drill hole KSH02 Extensometer measurements of the coefficient of thermal expansion of rock. SKB P-04-60, Svensk Kärnbränslehantering AB.

Åkesson U, 2004c. Drill hole KAV01 Extensometer measurements of the coefficient of thermal expansion of rock. SKB P-04-61, Svensk Kärnbränslehantering AB.

Åkesson U, 2004d. Drill hole KLX02 Extensometer measurements of the coefficient of thermal expansion of rock. SKB P-04-260, Svensk Kärnbränslehantering AB.

Åkesson U, 2004e. Drill hole KLX04 Extensometer measurements of the coefficient of thermal expansion of rock. SKB P-04-269, Svensk Kärnbränslehantering AB.

Åkesson U, 2004f. Drill hole KAV04 Extensometer measurements of the coefficient of thermal expansion of rock. SKB P-04-272, Svensk Kärnbränslehantering AB.

Appendix A

Probability plots of thermal conductivity per rock type

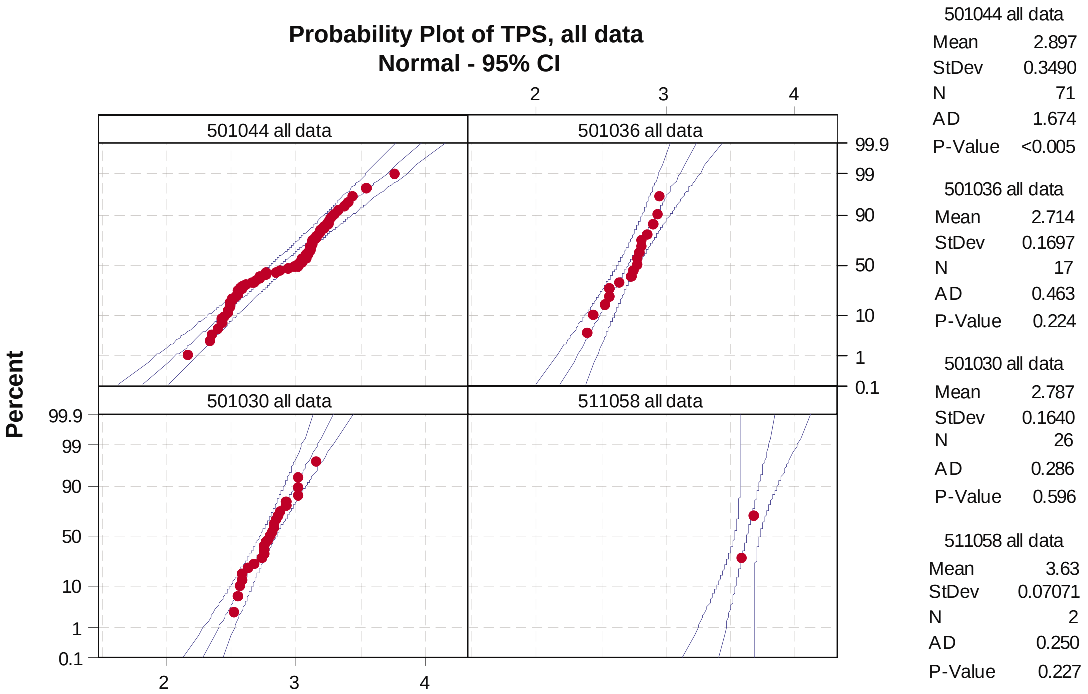

Figure A-1. *Probability plots of thermal conductivity from the TPS method for four rock types (normal distributions).*

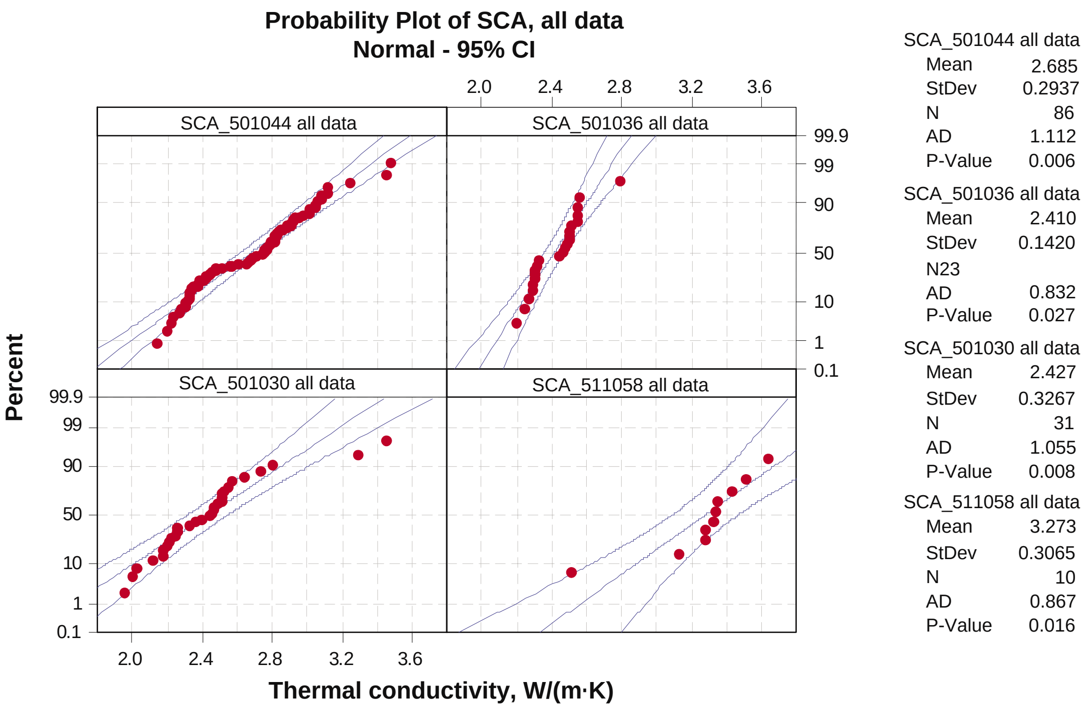

Figure A-2. *Probability plots of thermal conductivity from SCA values for four rock types (normal distributions).*

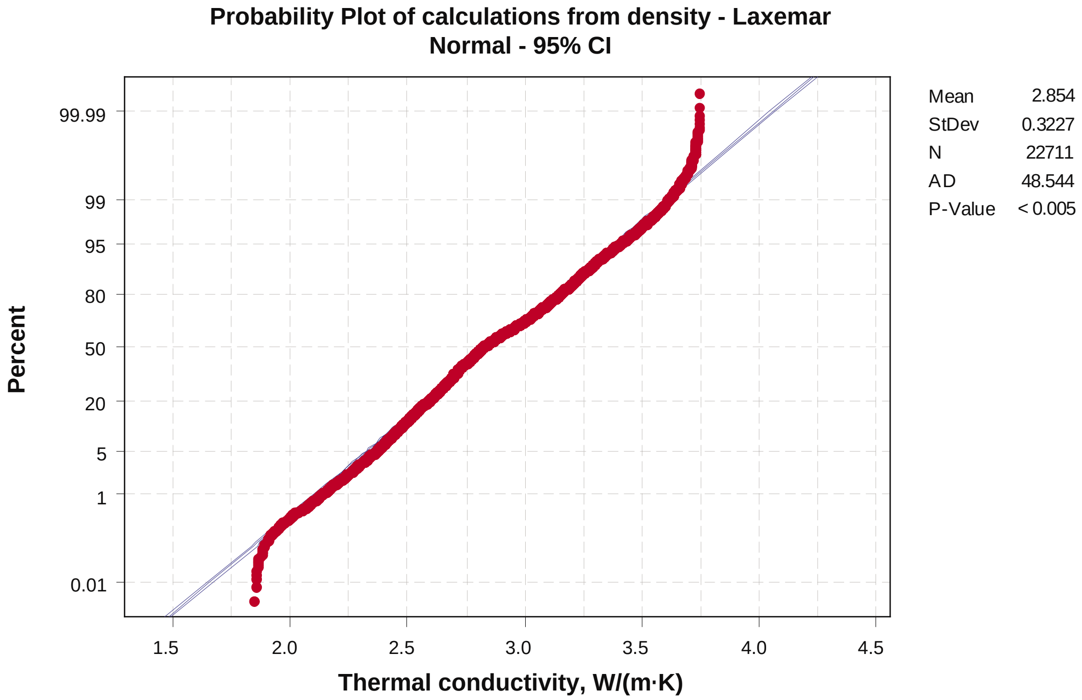

Figure A-3. *Probability plot of thermal conductivity from density logging for rock type Ävrö granite in the Laxemar subarea, normal distribution.*

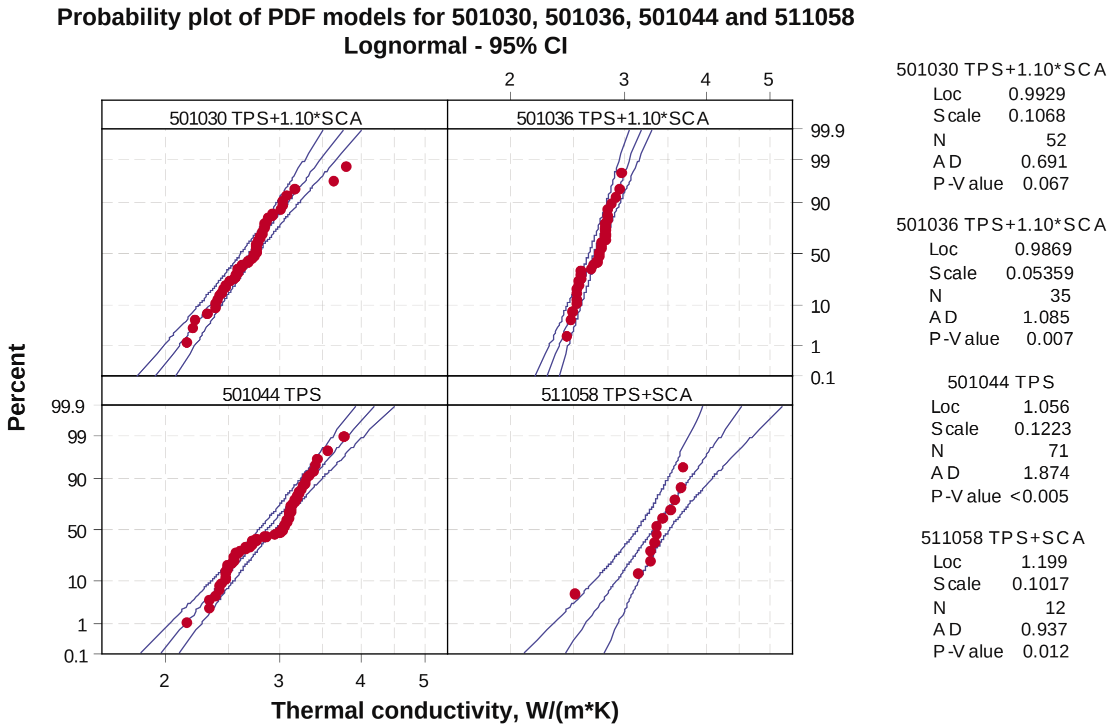

Figure A-4. *Probability plots (lognormal distributions) of thermal conductivity according to rock types. For rock types fine-grained dioritoid (501030) and quartz monzodiorite (501036) the SCA calculations have been corrected by a factor of 1.10.*

Probability plots of domain modelling results

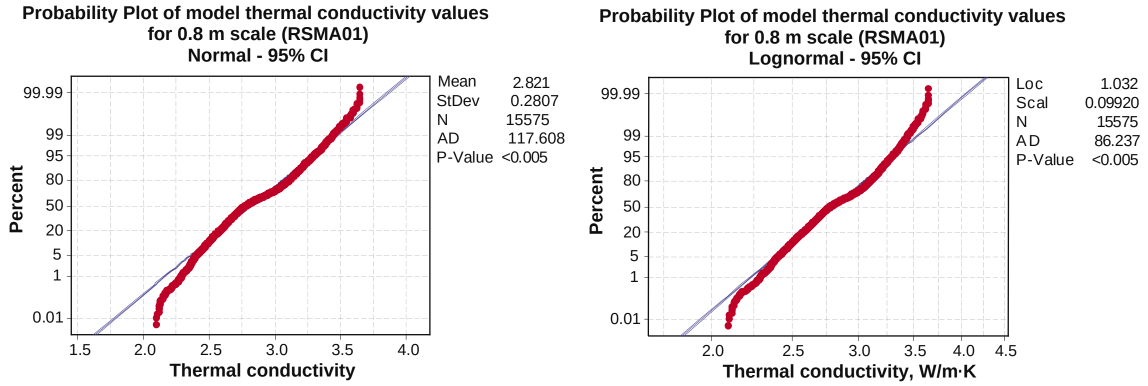

Figure B-1. *Probability plots of modelling results for 0.8 m scale for domain RSMA, (dominated by Ävrö granite), normal and lognormal distributions.*

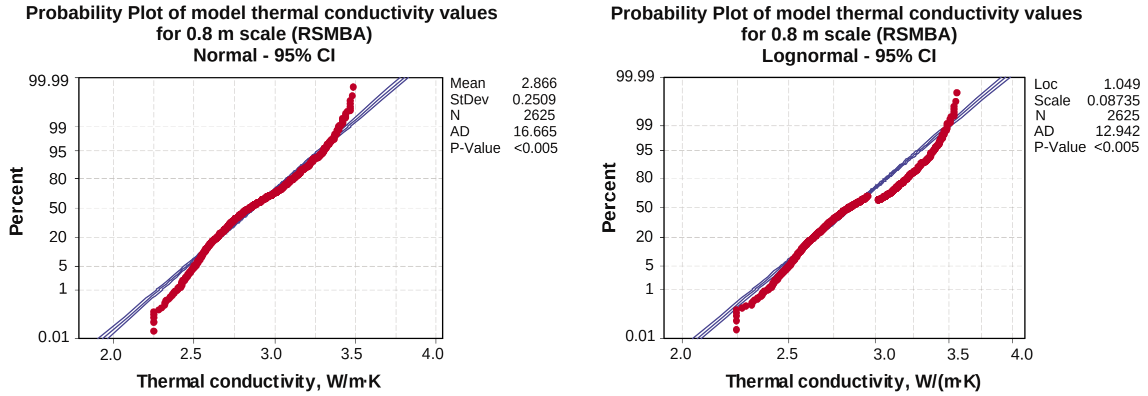

Figure B-2. *Probability plots of modelling results for 0.8 m scale in domain RSMBA03, normal and lognormal distributions.*

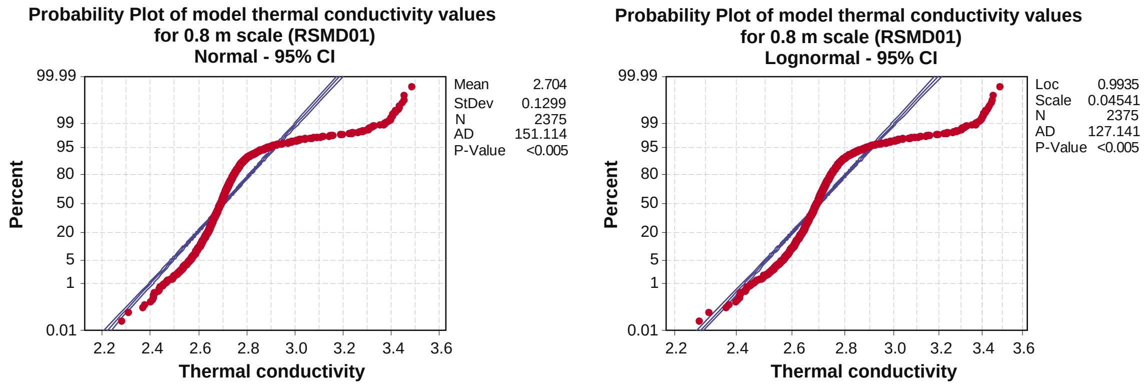

Figure B-3. *Probability plots of modelling results for 0.8 m scale in domain RSMD, normal and lognormal distributions.*

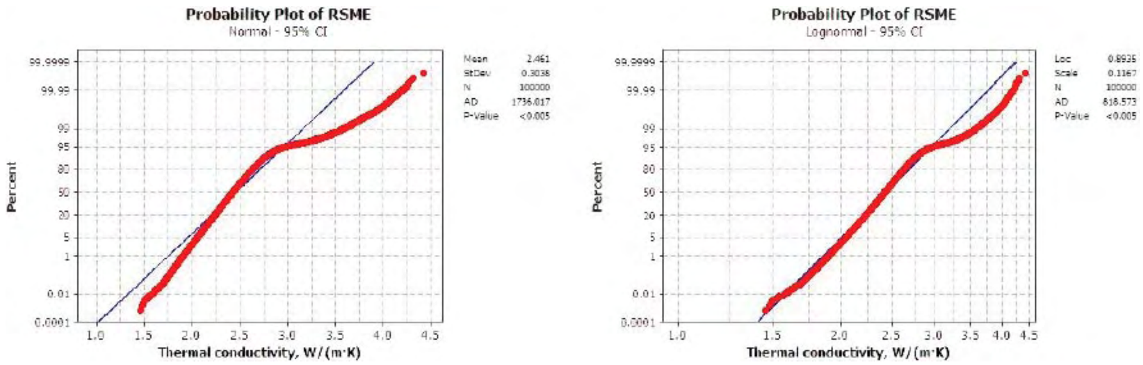

Figure B-4. *Probability plots of results from Monte Carlo simulation for domain RSME, normal and lognormal distributions.*

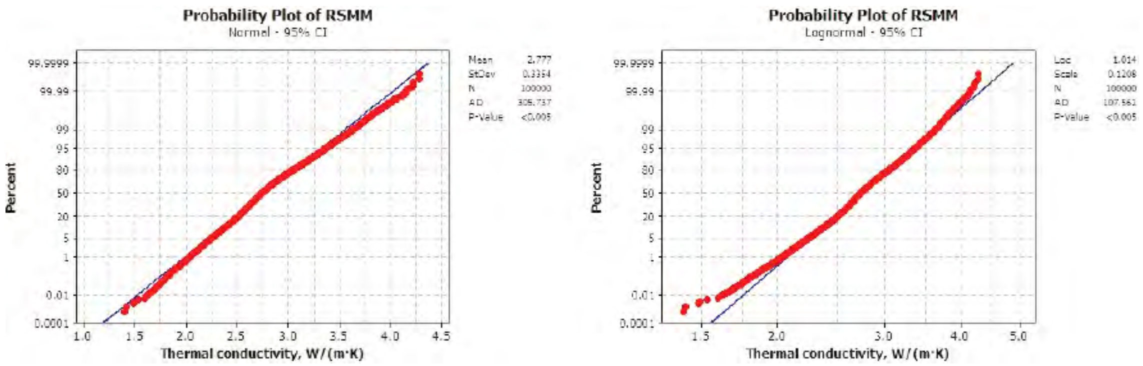

Figure B-5. *Probability plots of results from Monte Carlo simulation for domain RSMM, normal and lognormal distributions.*

Spatial variation of rock types – indicator variograms

The spatial distribution of different rock types can be modelled by indicator diagrams. Indicator variograms for Ävrö granite in domain RSMA (data from boreholes KLX01, KLX02, KLX03 and KLX04) are presented in Figure C-1. Segments/sections smaller than 1 m are included in the indicator variograms with a resolution of 5 cm.

The variance in such a variogram is calculated from indicators of “0” and “1”, where “0” indicates absence of the rock of interest and “1” indicates presences /Isaacs and Srivastava 1989/. In Figure C-1 indicator “1” indicates presence of Ävrö granite and “0” symbolises presence of a different rock type, i.e. the rock mass is classified in two categories. The variance on the y-axis is a measure of transition frequency between the two classes /Goovaerts 1999/. In other words, if two locations (A and B) in the borehole are selected, the indicator variance is the probability that either A or B, but not both, is located in Ävrö granite. The relatively low probability in Figure C-1 (~ 0.15) is because Ävrö granite dominates in the four boreholes, and is therefore much more likely that both A and B are located in Ävrö granite.

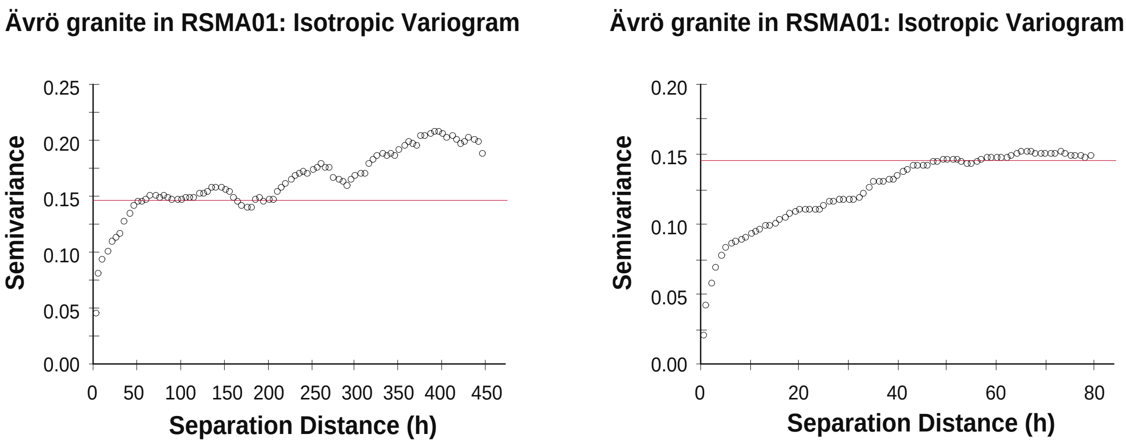

Figure C-1. *Indicator variogram of Ävrö granite (501044) in four boreholes in domain RSMA, separation distance 0–450 m and 0–80 m. The diagrams are constructed based on lithological classification (boremap).*

There is a strong correlation of the occurrence of Ävrö granite up to about 5 m. A lower, but still pronounced, correlation can be traced up to distances of about 50 m. Similar patterns were reported for Ävrö granite in boreholes in the Simpevarp subarea /Sundberg et al. 2005/.

Indicator variograms for quartz monzodiorite in domain RSMD (data from borehole KLX03) are presented in Figure C-2. There is a strong correlation of the occurrence of quartz monzodiorite up to about 20 m.

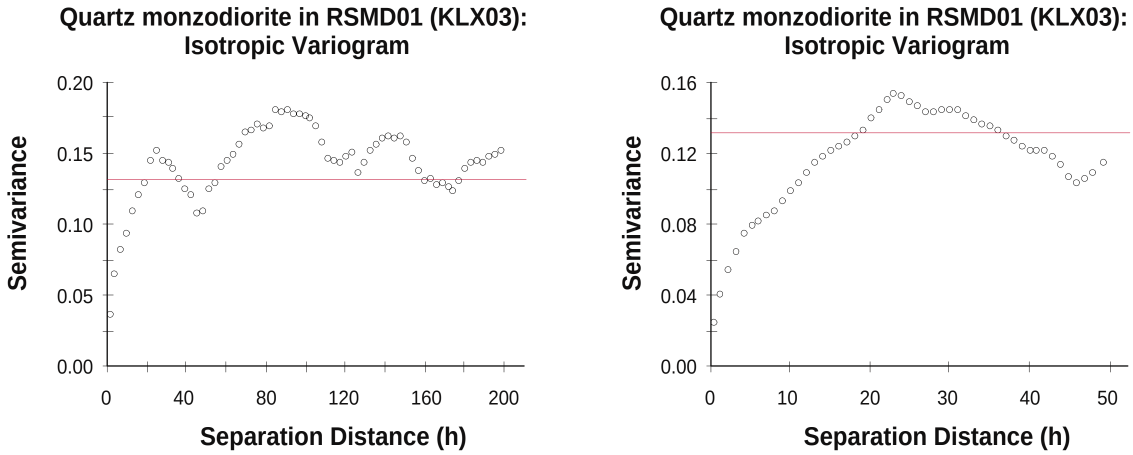

Figure C-2. *Indicator variogram of quartz monzodiorite (501036) in one borehole in domain RSMD, separation distance 0–200 m and 0–50 m. The diagrams are constructed based on lithological classification (boremap).*