R-07-42

Thermal site descriptive model

A strategy for the model development during site investigations – version 2

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September 2007

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ISSN 1402-3091
SKB Rapport R-07-42

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Preface

This thermal strategy report is an updated version of the original thermal strategy report /Sundberg 2003b/. The most important changes are concentrated to Chapter 3, which is totally revised, and Appendix A and B, which are new. A glossary of geostatistical terms has also been added. In addition, updating and modifications have been made in other parts of the report.

The main author of Chapter 1, 2, 4 and Appendix A are Jan Sundberg. Pär-Erik Back is the main author of Chapter 3 and the editor of the report. Appendix B was written by Pär-Erik Back and Lars Rosén, Sweco Viak.

A reference group has been connected to the project. The following persons have participated in the group: Johan Andersson, Rolf Christiansson, Lars O Ericsson, Harald Hökmark and Assen Simeonov. Professor Peter Dowd, University of Adelaide, is gratefully acknowledged for his support on geostatistical matters throughout the project. The authors would also like to express their gratitude for all fruitful comments on the report given by the reference group, Peter Dowd and Raymond Munier.

Summary

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 started during 2002. The site investigations shall provide the knowledge required to evaluate the suitability of investigated sites for a final repository. The interpretation of the measured data is made in terms of a site descriptive model (SDM) 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.

The deposited nuclear waste canisters will emit heat due to radioactive decay and the thermal conductivity of the rock will influence the temperature of the buffer surrounding the canister. It is important to describe the thermal conductivity distribution of the rock in order to design the repository considering the criterion of maximum buffer temperature. Characterisation of the thermal properties is referred to as thermal modelling.

This report presents a strategy for describing, predicting and visualising the thermal aspects of the site descriptive model. The strategy is an updated version of an earlier strategy applied in all SDM versions during the initial site investigation phase at the Forsmark and Oskarshamn areas. The previous methodology for thermal modelling did not take the spatial correlation fully into account during simulation. The result was that the variability of thermal conductivity in the rock mass was not sufficiently well described. Experience from earlier thermal SDMs indicated that development of the methodology was required in order describe the spatial distribution of thermal conductivity in the rock mass in a sufficiently reliable way, taking both variability within rock types and between rock types into account. A good description of the thermal conductivity distribution is especially important for the lower tail. This tail is important for the design of a repository because it affects the canister spacing. The presented approach is developed to be used for final SDM regarding thermal properties, primarily thermal conductivity.

Specific objectives for the strategy of thermal stochastic modelling are:

- Description: statistical description of the thermal conductivity of a rock domain.
- Prediction: prediction of thermal conductivity in a specific rock volume.
- Visualisation: visualisation of the spatial distribution of thermal conductivity.

The thermal site descriptive model should include the temperature distribution and thermal properties of the rock mass. The temperature is the result of the thermal processes in the repository area.

Determination of thermal transport properties can be made using different methods, such as laboratory investigations, field measurements, modelling from mineralogical composition and distribution, modelling from density logging and modelling from temperature loggings. The different types of data represent different scales, which has to be considered in the thermal modelling. Determination of temperature distribution in the rock mass and the geothermal gradient can be performed using temperature logging in boreholes. Other thermal data of interest is the thermal expansion of rock, which can be measured on core samples in the laboratory.

A methodology for the thermal site descriptive modelling is presented. It is an approach for assigning thermal properties to the rock mass in a rock domain, primarily thermal conductivity and heat capacity. The approach is based on stochastic simulation of the lithology and of the thermal conductivity. The main result is a set of equally probable realisations of thermal conductivity. Of special interest is the lower tail of the thermal conductivity distribution, which determines the canister spacing.

The methodology consists of the following steps:

1. Choice of simulation scale
2. Preparation of lithological data (hard data)
3. Defining Thermal Rock Classes (TRCs) within the rock domain
4. Preparation of thermal data (hard data)
5. Change of support
6. Specifying expert knowledge (soft data)
7. Estimating the spatial statistical structure of the TRCs
8. Stochastic simulation of TRCs
9. Estimating spatial statistical thermal model for each TRC
10. Stochastic simulation of thermal conductivity
11. Merging of realisations
12. Upscaling of simulation results
13. Presentation of results

The methodology is applied separately for each rock domain. The simulation scale (1) determines how lithological data (2) should be prepared and if a change of support (scale) (5) is required for the thermal data (4). The lithological data acquired from boreholes and mapping of the rock surface need to be reclassified into Thermal Rock Classes, TRCs (3). The main reason is to simplify the simulations; only a limited number of categorical classes can be handled in the simulations. The lithological data are used to construct models of the transition between different TRCs, thus describing the spatial statistical structure of each TRC (7). The result is a set of transition probability models that are used in the simulation of TRCs (8). The intermediate result of this first stochastic simulation is a number of realisations of the geology, each one equally probable.

Based on the thermal data, a spatial statistical thermal model is constructed for each TRC (9). It consists of a distribution model and a variogram model for each TRC. These are used in the stochastic simulations of thermal conductivity (10), resulting in a number of equally probable realisations of thermal conductivity. In the next step, the realisations of TRCs (geology) and thermal conductivity are merged together (11), i.e. each realisation of geology is filled with simulated thermal conductivity values. The result (13) is a set of realisations of thermal conductivity that considers both the difference in thermal conductivity between different TRCs and the variability within each TRC. If the result is desired in a scale different from the simulation scale, an upscaling can be performed (12). The result can be presented in a number of ways, for example as 3D illustrations, histograms and statistical parameters etc. The thermal realisations can also be used as input to design of a repository and for mathematical modelling of temperatures in and around a repository.

The main uncertainties are believed to be uncertainties in the spatial statistical structure of TRCs (7) and in the spatial statistical thermal models (9). If required, the methodology is continuously improved during the forthcoming construction and operation phases.

The main conclusions of the updated strategy for thermal modelling are:

- The statistical description of the thermal properties of a rock domain can be performed quantitatively using unconditional stochastic simulation. Almost any type of statistical property can be determined and its associated uncertainty estimated.
- Prediction of thermal properties in a specific rock volume can be performed using conditional stochastic simulation.

- Visualisation of the spatial distribution of thermal properties can be performed for both description and prediction.
- The methodology takes into account the spatial distribution of rock types (lithologies), including statistical properties and Markov properties, and the spatial variability of thermal conductivity within rock types.
- The proposed stochastic approach for thermal modelling has a high degree of transparency and flexibility. The mean reasons are the stepwise approach and the combination of lithological and thermal simulations, which allows for site-specific adjustments.
- The main uncertainties are believed to be uncertainties in the spatial statistical structure of TRCs and in the spatial statistical thermal models. In addition, the choice of simulation scale and associated uncertainties may have a significant impact on the result.
- The presented approach can be applied also for other properties than thermal.
- As a spin-off, the lithological realisations can be used to calculate statistics of the distribution of rock types. Such statistics can include lengths and volumes of rock bodies.

Sammanfattning

Svensk Kärnbränslehantering AB (SKB) ansvarar för hantering och slutförvar av det kärnavfall som produceras i Sverige. Platsundersökningar påbörjades under år 2002. Undersökningarna skall ge nödvändig kunskap för att utvärdera hur hållbara de undersökta platserna är för ett slutförvar. Tolkningen av mätdata sker i form av en platsbeskrivande modell (SDM) som omfattar geologi, bergmekanik, termiska egenskaper, hydrogeologi, hydrogeokemi, bergets transportegenskaper samt ytvattenekosystem. Den platsbeskrivande modellen är grunden för förståelsen av undersökningsdata och en bas för planering av förvarets utformning och för studier av byggbarhet, miljökonsekvenser och säkerhetsanalys.

Deponeringskapslarna med kärnavfall kommer att avge värme på grund av radioaktivt sönderfall och den termiska konduktiviteten hos berget kommer att påverka temperaturen i bufferten som omger kapslarna. Det är viktigt att prediktera den termiska konduktivitetsfördelningen hos berget så att förvaret kan utformas med hänsyn till kriteriet för maximal bufferttemperatur. Karaktäriseringen av termiska egenskaper benämns termisk modellering.

I denna rapport redovisas en strategi för beskrivning, prediktion och visualisering av den platsbeskrivande modellens termiska aspekter. Strategin är en uppdaterad version av en tidigare strategi som tillämpats för alla SDM-versioner under den inledande platsundersökningsfasen i Forsmark respektive Oskarshamn. Den tidigare metodiken för termisk modellering tog inte tillräcklig hänsyn till den spatiala korrelationen vid simuleringar. Resultatet blev att den termiska konduktivitetens variabilitet i bergmassan inte beskrevs tillräckligt väl. Erfarenheter från tidigare termiska SDMer indikerade att utveckling av metodiken krävdes för att beskriva den spatiala fördelningen av termisk konduktivitet i bergmassan på ett tillräckligt tillförlitligt sätt så att variabiliteten både inom en bergart och mellan bergarter beaktas. En bra beskrivning av den termiska konduktivitetsfördelningen är särskilt viktig för den låga svansen. Denna svans är betydelsefull vid konstruktion av ett slutförvar eftersom den påverkar kapselavståndet. Det redovisade angreppssättet har utvecklats för att kunna användas för slutgiltig SDM med avseende på termiska egenskaper, i första hand termisk konduktivitet.

Specifika syften med strategin för termisk modellering är:

- Beskrivning: statistisk beskrivning av den termiska konduktiviteten för en bergartsdomän.
- Prediktion: prediktion av termisk konduktivitet i en specifik bergvolym.
- Visualisering: visualisering av spatial fördelning av termisk konduktivitet.

Den termiska platsbeskrivande modellen ska omfatta temperaturfördelning, randvillkor och termiska egenskaper i bergmassan. Temperaturen är ett resultat av de termiska processerna i förvarsområdet.

Bestämning av termiska transportegenskaper kan göras med olika metoder, som exempelvis laboratorieundersökningar, fältmätningar, modellering från mineralsammansättning, modellering från densitetsloggar samt modellering från temperaturloggar. De olika typerna av data representerar olika skalor och detta måste beaktas i den termiska modelleringen.

Bestämning av temperaturfördelningen i bergmassan samt den geotermiska gradienten kan genomföras med hjälp av temperaturloggning i borrhål. Andra termiska data av intresse är längdutvidgning pga uppvärmning av berg, vilken kan bestämmas i laboratorium på prov från borrkärnor.

En metodik för termisk platsbeskrivande modellering presenteras. Den innebär ett angreppssätt för att tilldela bergmassan i en bergartsdomän termiska egenskaper, i första hand termisk konduktivitet och värmekapacitet. Angreppssättet baseras på stokastisk simulering av litologi

och termisk konduktivitet. Huvudresultatet är en samling lika sannolika realiseringar av termisk konduktivitet. Av särskilt intresse är den lägre svansen i den termisk konduktivitetsfördelningen, vilken är dimensionerande för kapselavståndet.

Metodiken består av följande steg:

1. Val av simuleringsskala
2. Behandling av litologi-data (hårda data)
3. Definition av termiska bergklasser (TRCer) i bergartsdomänen
4. Behandling av termiska data (hårda data)
5. Uppskalning från mätskalan (change of support)
6. Specificering av expertkunskap (mjuk data)
7. Bestämning av spatial statistisk struktur för TRCer
8. Stokastisk simulering av TRCer
9. Bestämning av spatial statistisk termisk modell för varje TRC
10. Stokastisk simulering av termisk konduktivitet
11. Sammanslagning av realiseringar
12. Uppskalning av simuleringsresultat
13. Presentation av resultat

Metodiken tillämpas separat för varje bergartsdomän. Simuleringsskalan (1) bestämmer hur litologi-data (2) ska behandlas och om uppskalning från mätskalan (5) är nödvändig för de termiska data (4). Litologi-data från borrhål och kartering av bergytor måste klassas om till termiska bergklasser, TRCer (3). Huvudskälet är att förenkla simuleringarna som bara kan hantera ett begränsat antal kategoriklasser. Dessa data används för att konstruera modeller av övergången (transitionen) mellan olika TRCer, vilka beskriver den spatiala statistiska strukturen för varje TRC (7). Resultatet är ett set modeller över transitionssannolikheterna. Dessa används vid simuleringen av TRCer (8). Resultatet från denna första stokastiska simulering är ett antal realiseringar av geologin, vardera lika sannolik.

Baserat på de termiska data konstrueras en spatial statistisk termisk modell för vardera TRC (9). En sådan består av en fördelningsmodell och en variogrammodell för varje TRC. Dessa används i de stokastiska simuleringarna av termisk konduktivitet (10), en för vardera TRC. Simuleringarna resulterar i ett antal lika sannolika realiseringar av termisk konduktivitet. I nästa steg slås de geologiska och de termiska realiseringarna samman (11), dvs. varje realisering av geologin (TRCer) fylls med simulerade termiska konduktivitetsvärden. Resultatet (13) är en samling realiseringar av termisk konduktivitet som beaktar både skillnaden i termisk konduktivitet mellan de olika TRCerna och variabiliteten inom en TRC. Om resultatet önskas i en annan skala än simuleringsskalan kan en uppskalning göras (12). Resultatet kan presenteras på en mängd olika sätt, t.ex. som illustrationer i 3D, histogram och som statistiska parametrar etc. De termiska realiseringarna kan även användas som input till utformning av ett förvar samt för matematisk modellering av temperaturer i och omkring förvaret.

De viktigaste osäkerheterna bedöms vara osäkerheter i den spatiala statistiska strukturen för TRCer (7) samt i de spatiala statistiska termiska modellerna (9). Om det visar sig vara nödvändigt kommer metodiken löpande att förbättras under kommande konstruktions- och driftsfaser.

De huvudsakliga slutsatserna i den uppdaterade strategin för termisk modellering är:

- Den statistiska beskrivningen av termiska egenskaper för en bergartsdomän kan genomföras kvantitativt genom okonditionerad stokastisk simulering. I stort sett vilken statistisk egenskap som helst kan bestämmas samt osäkerheten som är kopplad till denna.

- Prediktion av termiska egenskaper i en specifik bergvolym kan utföras med konditionerad stokastisk simulering.
- Visualisering av den spatiala fördelningen av termiska egenskaper kan utföras för både beskrivande och predikterande simuleringar.
- Metodiken beaktar den spatiala fördelningen av bergarter (litologi), inklusive statistiska egenskaper och Markov-egenskaper, men även den termiska konduktivitetens variabilitet inom en bergart.
- Det föreslagna stokastiska angreppssättet för termisk modellering medför en hög grad av transparens och flexibilitet. Huvudorsaken till detta är den stegvisa arbetsgången och kombinationen av litologiska och termiska simuleringar, vilket möjliggör platsspecifika anpassningar.
- De viktigaste osäkerheterna bedöms vara osäkerheter kopplade till spatial statistisk struktur för TRCer samt spatiala statistiska termiska modeller. Dessutom kan valet av simuleringsskala och osäkerheter kopplade till denna ha en signifikant påverkan på resultatet.
- Det presenterade angreppssättet kan också tillämpas på andra egenskaper än de termiska.
- Som spin-off kan de litologiska realiseringarna användas för att beräkna statistik på bergartsförekomster. Statistiken kan omfatta längder och volymer på bergartskroppar.

Glossary

The glossary is mainly developed for Chapter 3.

Categorical variable is a discrete variable that has a limited set of classes, e.g. Thermal Rock Classes (TRCs).

Change of support, see upscaling.

Conditional simulation is a type of simulation where actual observations or measurements are honoured, i.e. the simulated value in a cell will be equal to the measured value.

Cumulative Distribution Function (CDF) is a function describing the statistical distribution of a population. The value of the y-axis is the proportion of values that is lower than the x-value, i.e. the scale of the y-axis is from 0 to 1 (0% to 100%).

Declustering is a geostatistical technique to handle data that occur in spatial groups, so called clusters. Each data value is given a weight and clustered samples are given less weight than others. The weights are considered when the statistics are calculated, resulting in mean and variance that are more representative.

Gaussian simulation is a type of stochastic simulation where simulated values follow a Gaussian (normal) distribution. If measurements are not Gaussian, a Gaussian transformation must first be applied.

Histogram is a graph that shows the distribution of the occurrence of different values, separated into a finite set of classes.

Indicator simulation is a stochastic simulation technique for simulation of different classes of a categorical variable. The classes are defined by indicators and cut-offs between the classes. Indicator variogram models are used to simulate the spatial occurrence of the different classes.

Kriging (linear) is an interpolation method, resulting in the best linear unbiased estimator. Under correct assumptions, the method gives a mean error equal to 0 and minimises the variance of the errors. Kriging is often the best option for making prognosis of mean properties (estimation) but it is not a good option for characterising uncertainty because of its smoothing effect; compare *stochastic simulation*.

Lag is the separation distance between classes of spatial data. In the variogram, the lag is plotted on the x-axis. The spatial correlation will usually decrease when the lag increases.

Markov chains describe the change of state in a system over space (or time). The changes of state are called transitions. The Markov property means that the conditional probability distribution of the state depends only on the state of the neighbouring cell. Markov chains can be used for calculating transition probabilities of categorical variables.

Nugget is the (apparent) intersection of the variogram with the y-axis, i.e. the variance at separation distance (lag) zero. It results from measurement errors and/or micro-variability at scales smaller than the sample support, appearing in the form of white noise /Journel and Huijbregts 1978/.

Probability Density Function (PDF) is a function describing the statistical distribution of a population. The value of the y-axis is the probability density, which is the derivative of the Cumulative Distribution Function (CDF), i.e. the maxima and minima of a PDF correspond to the inflection points in a CDF.

Range is a distance representing the zone of influence of a sample. It is the distance on the x-axis where the variogram reaches a more or less pronounced plateau.

Rock domain is a region of the rock mass for which the properties can be considered essentially the same in a statistical sense. Several *rock units* are assembled into a rock domain. In the thermal modelling, properties are modelled for the different rock domains.

Rock unit is term used for a volume of rock judged to have a reasonably statistically homogeneous distribution of lithology (rock types) and fracturing statistics. It may contain several different rock types judged to be similar. A rock unit may also contain small-scale inclusions of very different rock types. Each rock unit is defined by its location and is described in terms of rock type distribution and fracture statistics.

Sill represents the variance beyond the zone of influence, i.e. the value on the y-axis of the variogram at the plateau.

Simulation domain is the rock volume that is simulated, i.e. the size of each realisation from a stochastic simulation. The simulation domain should not be interpreted as rock domain; they do not necessary coincide.

Spatial correlation indicates the strength and direction of a linear relationship between two spatially separated data values. Two values are considered positively correlated if an increase in one value results in an increase of the other value. Spatial thermal conductivity data are positively correlated, up to the range.

Stochastic simulation is the general term for techniques for assigning random values to stochastic variables, according to a model describing the random properties. Spatial stochastic simulation is used when the values should be distributed in space, which requires a spatial model, e.g. a variogram model. It can be performed on continuous variables (such as thermal conductivity) or categorical variables (such as thermal rock classes). Stochastic simulation is used when the uncertainty of a parameter must be quantified (uncertainty analysis or risk analysis); compare *Kriging*.

Support is the term used for measurement scale in geostatistical nomenclature. It is the volume, shape, and orientation that a measurement represents /Starks 1986/.

Thermal Rock Class (TRC) is a concept defined in this report. There are many rock types but simplifications are required in the stochastic simulations and therefore rock types with similar thermal conductivity are classified as a single thermal rock class. This is performed by considering the importance of a rock type from a thermal point of view, the spatial statistics of thermal conductivity, and the geological aspects for each rock type.

Transition probability is the probability of a change, a transition, between two states of a categorical variable. Example: The probability of transition from Ävrö granite to Quartz monzodiorote.

Unconditional simulation is a method that distributes simulated data spatially without honouring measurements at specific locations.

Upscaling, or change of support, refers to the change of the scale of data or simulated values. The upscaling results in a different statistical distribution (change in variance and in the mean). Generally, the variance is reduced when the scale increases.

Variogram is a graph that describes how the variance changes as a function of separation distance (lag). A variogram illustrates the spatial correlation. A variogram model can be fitted to the experimental variogram to model the spatial correlation.

Contents

1 Introduction

1.1 Background

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 started during 2002 /SKB 2000a/. The site investigations are carried out in different stages /SKB 2001/ and shall provide the knowledge required to evaluate the suitability of investigated sites for a final repository. The technique for long-term storage of spent nuclear fuel is developed at the Äspö Hard Rock Laboratory.

The interpretation of the measured data is made in terms of a site descriptive model (SDM) covering geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties of the rock and surface ecosystems /SKB 2001/. 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.

The deposited nuclear waste canisters will emit heat due to radioactive decay and the thermal conductivity of the rock will influence the temperature of the buffer surrounding the canister. A low thermal conductivity leads to a larger required distance between the canisters than in the case of a high thermal conductivity. It is important to describe the thermal conductivity distribution of the rock in order to design the repository for a suitable buffer temperature. Characterisation of the thermal properties is referred to as thermal modelling. In this work, both measurements and simulations are performed.

This report presents a strategy for describing, predicting and visualising the thermal aspects of the site descriptive model. The strategy is an updated[1] version of an earlier strategy applied in all SDM versions during the initial site investigation phase at the Forsmark and Oskarshamn areas; see /Sundberg 2003b/. The previous methodology for thermal modelling is described in detail in /Sundberg et al. 2005c/. It did not take the spatial correlation fully into account during simulation, which resulted in underestimation of the variance after upscaling. Subjective adjustments were made in order to correct for the too large variance reduction during upscaling. In addition, only one realisation was considered, i.e. the boreholes, and upscaling was performed in 1D only. The result was that the variability of thermal conductivity in the rock mass was not sufficiently well described. Experience from earlier thermal SDMs /Sundberg et al. 2005ab, 2006, Wrafter et al. 2006/ indicated that development of the methodology was required in order describe the spatial distribution of thermal conductivity in the rock mass in a sufficiently reliable way, taking both variability within rock types and between rock types into account. A good description of the thermal conductivity distribution is especially important for the lower tail. This tail[2] is important for the design of a repository because it affects the canister spacing. These are the main reasons for developing the methodology for thermal modelling.

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[1] Such updating is part of SKB's overall modelling strategy.

[2] The lower tail must be characterised in a proper way without the assumption of a normal distribution. Previous work indicates that the statistical distribution of thermal conductivity values at rock domain level is far from normally distributed, which means that the mean and the standard deviation are not sufficient to characterise the distribution. The reason for the deviation from a normal distribution is that the rock domain consists of several different rock types with widely different thermal conductivities. No common statistical distribution can be expected to fit the distribution of thermal conductivity at the rock domain level, even though the distribution for a particular rock type may be close to normal.

The aim of this updated strategy is to enhance how the spatial variability in lithology and thermal transport properties is handled within the rock domains that have been identified in the geological modelling. This provides a better basis for characterisation and upscaling of these properties.

The approach presented in this report is developed to be used for the final SDM regarding thermal properties, primarily thermal conductivity. The strategy will also be used during later construction phase but additional revisions may then become necessary.

1.2 Objectives and scope

1.2.1 General objectives

The objective of this report is to present a strategy for developing the Thermal Site Descriptive Model within the SKB Site Investigation Programme. General objectives in the Site Descriptive Modelling are:

- The strategy is developed for needs connected to siting and building of a KBS-3 type repository in crystalline rock, with focus on the conditions to be expected at the sites selected for site investigations /SKB 2000a/. The strategy should provide the site specific properties needed for design and safety assessment.
- The strategy should be adapted to the iterative and integrated character of the Site Investigation and Site Evaluation programme /SKB 2000b/. Descriptions should be consistent with those made in other disciplines (mainly geology).
- The strategy should allow full transparency of data gathering, management, interpretations, analysis and the presentation of results. The interpreted parameters should cover the entire model domain, not just in the proximity of measuring points. Spatial variability, as well as conceptual and data uncertainty due to sparse data, errors and lack of understanding should be handled and illustrated.
- The strategy should make use of experiences gained.

1.2.2 Specific objectives for thermal modelling

The aim of the thermal modelling is to model the thermal properties spatially for a defined rock mass, primarily a rock domain. The term “thermal properties” involves thermal conductivity, thermal diffusivity, heat capacity, temperature and the coefficient of thermal expansion. All these parameters are addressed in the strategy for estimating thermal properties (Chapter 2). The stochastic modelling in Chapter 3 is restricted to the parameter thermal conductivity. However, there is a relationship between thermal conductivity and heat capacity, which implies that also heat capacity can be characterised by this approach.

There are three specific objectives for the thermal stochastic modelling:

- Description: statistical description of the thermal conductivity of a rock domain.
- Prediction: prediction of thermal conductivity in a specific rock volume.
- Visualisation: visualisation of the spatial distribution of thermal conductivity.

The approaches to reach these objectives and the expected results are described in Section 3.2. In addition, the updated strategy should:

- take spatial variability within lithologies (rock types) into account,
- take the variability between lithologies into account,
- be able to handle measurements (hard data) representing different scales,

- handle uncertainties and, if possible, quantify them,
- make the methodology transparent and easy to understand.

The thermal properties and their estimation have to comply with requirements from design and safety assessment.

The result of applying the presented strategy in Chapter 3 is a set of equally probable realisations of thermal conductivity and heat capacity. These realisations can be used as input to design of a repository and for mathematical modelling of temperatures in and around a repository. In addition, from the lithological realisations it is possible to calculate statistics of the distribution of rock types.

1.3 Thermal properties and processes

1.3.1 Definitions

Thermal conductivity and heat capacity is needed to describe the thermal transport process. Thethermal conductivity, λ [W/(m·K)], describes the ability of a material to transport heat. The heat capacity denotes the capacity for a material to store thermal energy. The volumetric heat capacity, C [J/(m^3·K)], is the product of density, ρ, and specific heat capacity, c [J/(kg·K)].

The thermal diffusivity, κ [m^2/s], describes a material's ability to level temperature differences. It is defined as the ratio between thermal conductivity and volumetric heat capacity:

$$\kappa = \lambda/(\rho \cdot c) \tag{1-1}$$

The geothermal gradient [°C/m] describes the temperature increase versus depth.

The geothermal heat flow, q [W/m^2], describes the flow of heat, detected on the ground surface, from the inner part of the Earth. The natural geothermal heat flow in Sweden is mainly a vertical process and governed by the equation:

$$q = -\lambda \cdot \left(\frac{dT}{dz} \right) \tag{1-2}$$

where dT/dz is the geothermal gradient, the temperature change as a function of depth below the ground surface.

The internal heat production [µW/m^3] is defined as the heat produced within the rock mass due to nuclear decay of primarily Uranium, Thorium and Potassium.

The coefficient of thermal expansion [m/(m·K)] describes the linear expansion due to thermal influence.

1.3.2 Thermal properties of rock and other parameters

The thermal site descriptive model should include the temperature distribution, boundary conditions and thermal properties of the rock mass. The temperature is the result of the thermal processes in the repository area. The boundary conditions are represented by the geothermal heat flow and by temperature and climatic conditions at the ground surface.

The thermal properties and parameters are listed in Table 1-1 together with some initial suggestions for acceptable values of uncertainty.

The thermal properties are measured for the intact rock, often as small-scale measurements. Discontinuities in the form of cracks influence the thermal properties at larger scales. However, this influence is supposed to be small and is therefore neglected during upscaling of the thermal properties.

Table 1-1. Listing of thermal properties and parameters that can be described by the thermal model, including some initial suggestions for acceptable uncertainty values. For definitions, see Section 1.3.1.

Parameter	Unit	Suggestion for acceptable uncertainty
Thermal transport properties		
Thermal conductivity	W/(m·K)	± 10% if λ > 3 W/(m·K) ± 5% if 2.6 < λ < 3 W/(m·K) < ± 5% if λ < 2.6 W/(m·K)
Heat capacity	J/(m^3·K) or J/(kg·K)	± 10% but better accuracy is suitable for low λ
Thermal diffusivity	m^2/s	
Temperature		
Temperature in the rock mass	°C	± 0.5°C
Temperature gradient	°C/m	
Boundary conditions		
Geothermal heat flow	W/m^2	± 10%
Temperature and climate conditions at the ground surface	°C	± 10%
Other thermal properties		
Internal heat production in the rock	μW/m^3	± 20%
Thermal expansion of rock	m/(m·K)	± 20%
Other relevant properties		
Density and porosity	kg/m^3 and %	± 5%

1.3.3 Thermal processes

The temperature and the temperature distribution are central for the design of the repository and also influence rock mechanical stability, groundwater flow, biological activity and chemical reactions.

Natural temperature field

The natural temperature field in the rock is a function of the following factors:

- The temperature variation at the ground surface.
- Heat flow from the interior of the Earth and internal heat production in the rock mass.
- Heat transport by conduction and convection in soil, rock and fracture zones.

The natural temperature field in the ground is a function of boundary conditions, internal heat production and thermal transport properties in the rock mass.

The boundary conditions at the ground surface consist of variations in the climate conditions on the ground surface (air temperature, snow, radiation etc) in different time scales. The air temperature varies in time and with the geographic location. For a time-scale of about 10 years, the mean temperature at a certain location is relatively constant. Climate variations influence the mean temperature in a larger time perspective. It is only the large-scale variations that will influence the temperature at the depth of a repository.

The lower boundary condition is the heat flow at great depth from the interior of the Earth. The temperature is also influenced by small amounts of heat generated by radioactive decay of Uranium, Thorium and Potassium in the rock itself.

In the rock mass, the thermal transport mainly results from conduction and locally, in fracture zones, of convection due to ground water movement. Heat transport through radiation can be neglected.

The equation of heat conduction in a homogeneous and isotropic media can be written as:

$$\partial^2 T/\partial x^2 + \partial^2 T/\partial y^2 + \partial^2 T/\partial z^2 = (1/\kappa) \cdot (\partial T/\partial t) \qquad (1\text{-}3)$$

where

T = temperature

t = time

κ = thermal diffusivity. $\kappa = \lambda/(\rho \cdot c)$, i.e. the thermal diffusivity is equivalent to the ratio between the thermal conductivity (λ) and the product of density (ρ) and specific heat capacity (c).

x, y, z = coordinates in space.

Building the repository

The natural temperature field will be disturbed by the building of the repository, related to ventilation and lighting work etc. When the canisters containing nuclear waste are deposited in the repository, the generated heat of the deposited canisters, due to radioactive decay, will disturb the original temperature field. The temperature increase and subsequent cooling-off cause a volume change of the rock mass due to thermal expansion. The long-term behaviour of the thermal function of the repository is dependent on the declination of the generated heat, future changes in boundary conditions and the temperature dependence of the thermal transport properties in the rock mass.

The local temperature field in the repository depends on thermal properties of the rock and backfill, and the generated heat of the canisters due to decay. The layout of the repository is mainly dependent on the local temperature field.

1.3.4 Relevant scales

Introduction

The thermal properties vary depending on the scale of observation. Observation scales may range from millimetres or less, up to 1,000 m or more. Heterogeneities exist at the whole spectrum of scales and the resulting variability must be handled. A common approach is to use effective values to characterise the thermal conductivity at a particular scale (or as a mean value for anisotropic rock). The effective value for a larger scale than the measurements represents can be approximated by calculations, i.e. upscaling. The geometric mean is a good approximation of the effective thermal conductivity for a larger scale. The Self Consistent Approximation (SCA) method is theoretically the appropriate method of upscaling in 3D; see Appendix A. However, the difference compared to the geometric mean is often small for thermal conductivity in rock.

The statistical parameters of the distribution of thermal conductivity values are of course affected by the upscaling. The mean of the distribution is generally affected only to a small extent. However, the variance and standard deviation are usually reduced when the scale (support) is increased. This is because the variability at the measurement scale is evened out when the rock is observed at a larger scale. This implies that the shape of the thermal conductivity distribution will depend on the scale of observation.

Scale of laboratory determination of thermal properties

Rock forming minerals have different thermal properties; see i.e. /Sundberg 1988/. The different minerals exist at a micro- or millimetre scale. Thus, there is a rather large variation in thermal properties at this scale. If the rock is fine-grained, isotropic and homogeneous, the variations have to a large degree been averaged out at the cm scale. Determinations of thermal properties in the laboratory are often made at this scale. However, even for a homogeneous rock type there is always a variation in properties due to chemical variations in the original magma. This variation may occur at the 1–100 m scale.

If the rock is relatively homogeneous, variation of thermal conductivity at one scale is averaged out at a certain distance (a larger scale). If the rock is anisotropic and heterogeneous, a larger variation will exist at the small scale but not necessarily at the larger scale.

Preliminary, the following scales are believed to be relevant:

- 0.0001–0.001 m for mineral analyses.
- 0.005–0.05 m for determination of thermal properties in laboratory.

Scale of determination of thermal properties by field measurements

Measurements of thermal properties in the field have been conducted using methods resulting in thermal data for different scales. The methods include thermal response test, multi-probe measurements, measurements of thermal gradient, density logging, and single probe measurements in boreholes. The data are representing the following scales:

- Single- or Multi-probe measurements (0.2–1 m), depending on the time of measurement and temperature sensor configuration.
- Density logging (0.2 m).
- Thermal response test (5–100 m).

Scale of thermal processes in a repository

The thermal function of a repository can be studied at different scales, exemplified in Figure 1-1. In order to describe the influence from natural climatic conditions above ground, on the thermal conditions in a repository, mean values and deviations of thermal transport properties for the whole rock mass can be representative. The sensitivity of the canister temperature for changes in the thermal properties is highest for the area close to the canister. It is therefore of special interest to analyse the variation in thermal properties in the rock mass at the scale 1–20 m (canister deposition scale and up to tunnel scale). Small scale variations, below 1 m, in thermal rock properties are not influencing the bentonite temperature /Sundberg et al. 2005c/.

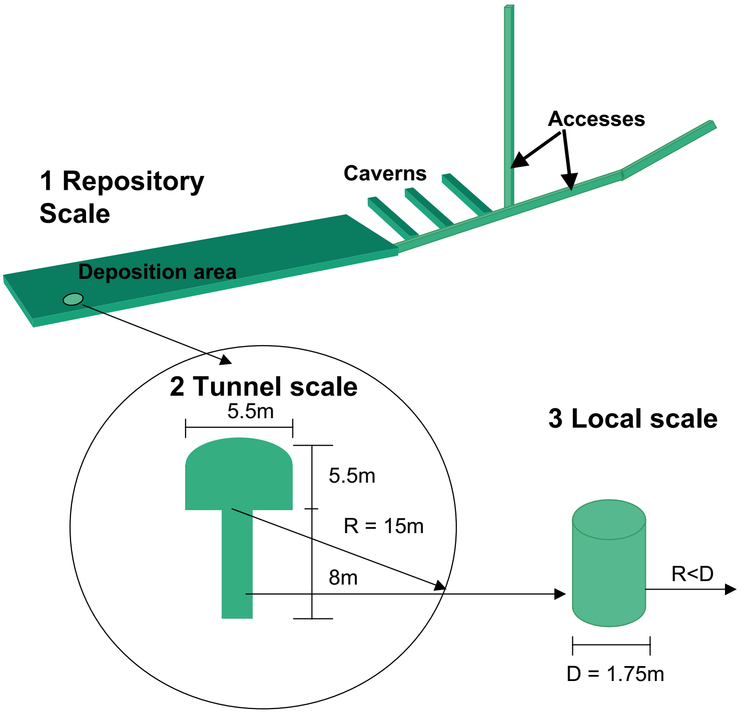

Figure 1-1. *Illustration of the various scales of importance for rock mechanics considerations for siting and constructing a KBS-3 repository, from /Andersson et al. 2002/.*

Preliminary, the following scales are believed to be relevant:

- 1–10 m for the thermal function of the canister (canister scale or local scale).
- 10–100 m for the thermal function of the tunnel (tunnel scale).
- 100–1,000 m for the thermal function of the whole repository (repository scale).

The "global" temperature field around a repository mainly depends on the time-dependent generated heat, boundary conditions, initial temperature conditions and mean values of large-scale thermal transport properties. The thermal processes at this scale are quite slow and insensitive to local variations in the thermal properties. The demands for high accuracy in the thermal property distribution are lower compared to the local scale.

The local temperature field is of primary concern for the design of a repository. The current design criterion is specified as the maximum temperature allowed in the bentonite buffer outside the canisters /SKB 2006/. A low thermal conductivity leads to larger distances between canisters than in the case of a high thermal conductivity.

The sensitivity in canister temperature to changes in the thermal properties is highest for the area closest to the canister. It is therefore of special interest to analyse the thermal impact on the canister if there is a variation in the thermal properties in the rock mass at the canister scale, 1–10 m, that will influence the canister temperature.

/Ageskog and Jansson 1999/ carried out heat propagation studies for a repository in three different rock types. /Probert and Claesson 1997/ made temperature field modelling with time dependent heat sources for the KBS-3 repository. /Hökmark and Fälth 2003/ made design calculations on the influence of canister spacing and thermal conductivity on the maximum canister temperature.

In /Sundberg 2003a/, local scale mathematical simulations were made of the sensitivity in canister temperature due to variations in thermal properties within rock types and between two different outcrops of rock types, A and B. The simulations show that variations in the thermal conductivity at a scale up to about 0.5–1.0 m is averaged out and have small influence on the canister hole temperature. Larger blocks at a scale of 5–10 m with different thermal conductivity have a significant influence on the deposition hole temperature. With high and well-defined thermal properties in the tunnel area there is still a large influence on canister temperature if low conductive rock is present outside the tunnel. The thermal behaviour in canister-tunnel scale is more influenced by variations in the thermal conductivity than in the heat capacity.

In order to analyse the lower scale for which variations of thermal conductivity is significant for the temperature on the canister, a numerical study based on rock thermal conductivity distribution have been made /Sundberg et al. 2005c/. They found that the spatial variability started to have an influence on the canister temperature at a scale as small as 1 m and that the influence increased approximately linearly up to 10 m (Figure 1-2). Consequently, the maximum temperature is influenced by thermal conductivities for a range of scales. The characteristic scale would be in the order of 2–5 m, which is logical considering the dimensions of the canister and the dominating role of the contribution of the local canister to its own temperature.

1.3.5 Uncertainty and required confidence

The properties must be determined and upscaled with such a degree of certainty and resolution that the temperature field around the repository can be described with sufficiently high degree of confidence and security with regard to the maximum temperature allowed on the bentonite buffer outside the canisters.

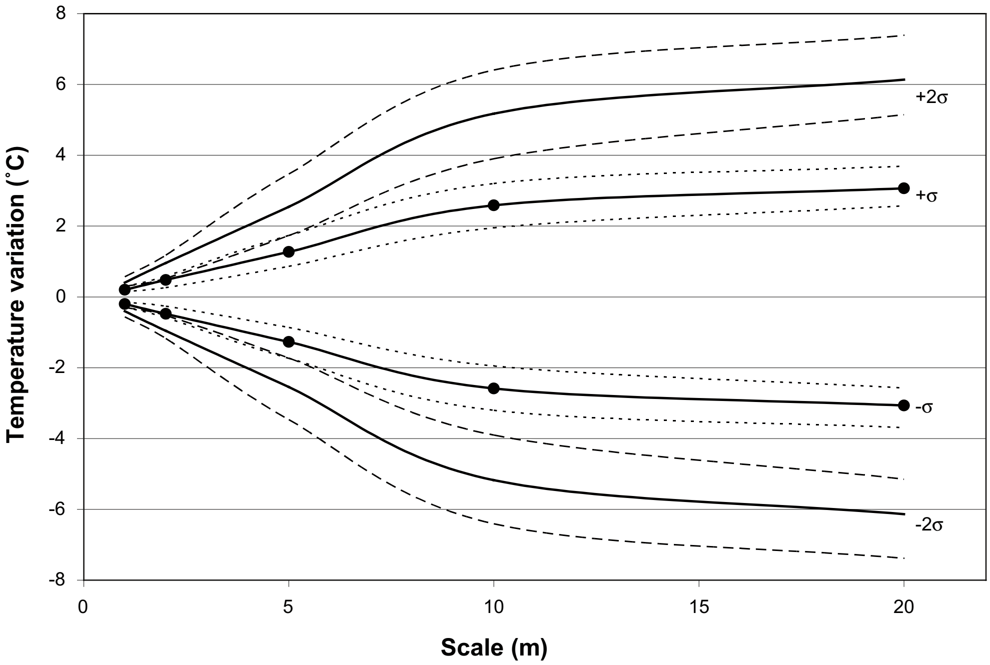

Figure 1-2. *Simulated canister temperature variations at one and two standard deviations based on average values for each scale. Thermal conductivity values are randomly assigned from a normal distribution for each scale (mean: 2.8 W/(m·K), std: 0.35 W/(m·K). The dotted lines show the temperature variation based on the min and max standard deviation /Sundberg et al. 2005c/. The temperature variation is affected by thermal conductivities for a range of scales. Note that the temperature variation at larger scales is a result of the simulation approach.*

There are different kinds of uncertainties that influence the description of thermal properties of rock, most importantly:

- Inaccuracy and imprecision in the estimations of thermal properties.
- Natural variations in the properties for the intact rock, including anisotropy.
- The spatial distribution of rock properties.

The first type of uncertainty, inaccuracy and imprecision in the estimations of thermal properties, results from data uncertainties (Section 2.6) and uncertainties in the modelling approach (Section 3.6).

The uncertainty can be estimated from statistical variation and from the validity of other interpretations based on measurement information. The confidence of a value can also be estimated when comparing results from later investigations with earlier investigations. Good agreement between estimated and measured values suggests that the confidence in the parameters and the model is reasonable.

The acceptable uncertainty for each parameter depends on the absolute value of the parameter and the required confidence of that parameter.

The requirements on the confidence are higher for the lower tail of the thermal conductivity distribution, especially if the absolute values are relatively low, since this affect the minimum distance between canisters; see e.g. SR-Can /SKB 2006/.

1.4 Modelling approach

1.4.1 Model requirements

The thermal modelling approach is a part of the general approach to site descriptive modelling. The model should meet the following requirements in order to be a basis for design and safety assessment:

- Ensure that necessary properties, parameters and processes have been included.
- Allow full transparency in primary data, data flow, evaluation and presentation.
- Provide 3D simulated thermal data for the entire domain as well as statistical distribution of thermal properties.

1.4.2 General approach to site descriptive modelling

The general site investigation programme describes both investigation methods and execution programmes for the different disciplines /SKB 2001/. Figure 1-3 shows the flow of information from site investigations to site descriptive models for various disciplines, eventually converging

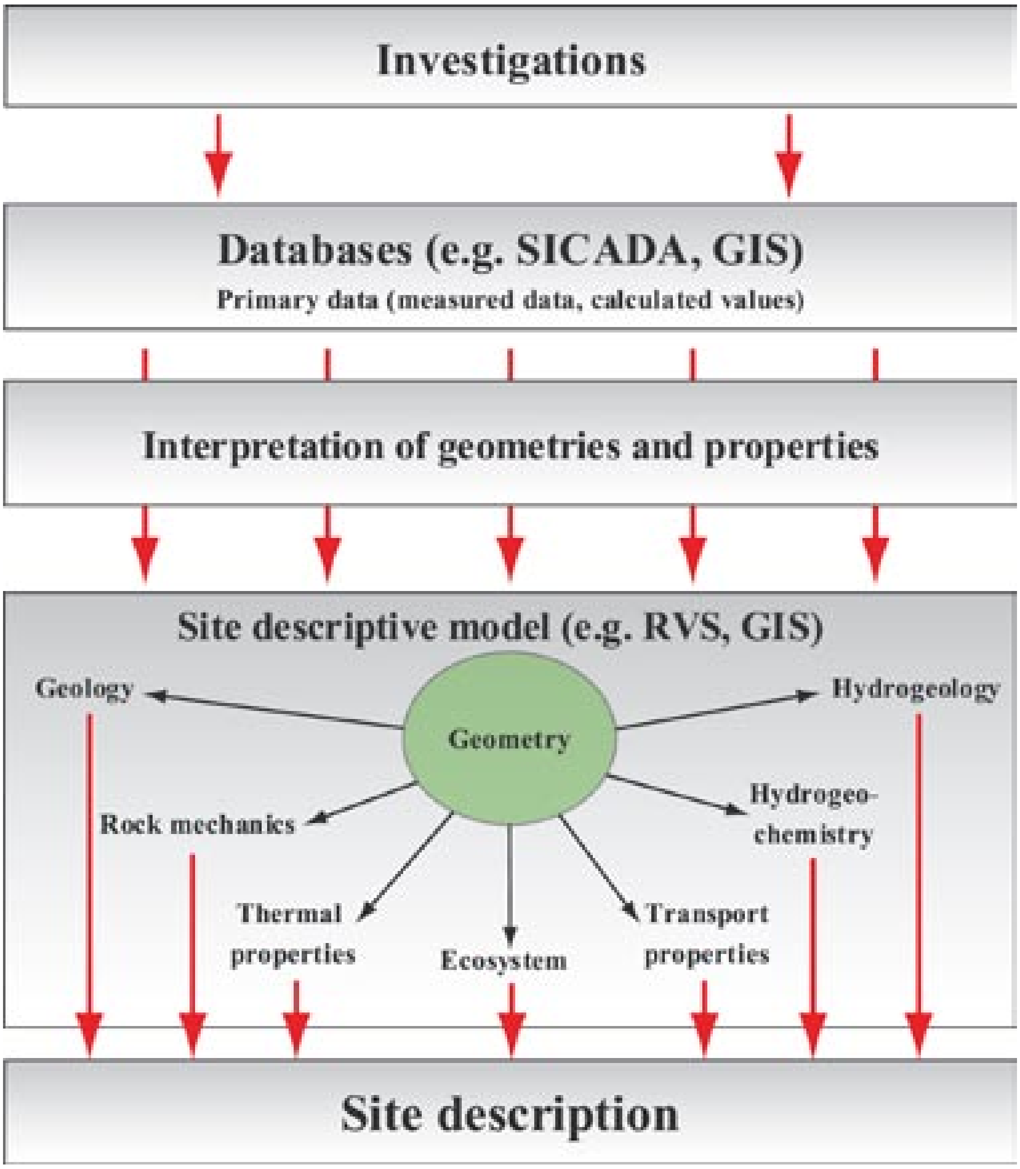

Figure 1-3. The information flow from site investigations to site description and associated databases.

into a consistent site description. The information flow in the figure has been simplified. In reality, there is substantial feedback to earlier stages in the chain and exchanges of information between the different disciplines. The investigations, comprising evaluation and modelling, are executed in different stages. Design work and safety assessment analyses are carried out parallel to the information flow in the figure, and allow feedback to all stages.

In /SKB 2001/ a summary of site descriptive models for different disciplines are presented. The summary of the thermal site descriptive model is given in Table 1-2. The specific approach to thermal modelling is described in Chapter 3.

Table 1-2. Brief presentation of purpose and content of the Thermal Site Descriptive Model; from /SKB 2001/.

Purpose of model

The parameters included in the model shall serve as a basis for design and safety assessment and the analyses performed in these steps. The model shall describe, for a given investigated volume, the initial temperature conditions and the distribution of thermal properties in the rock volume.

Process description

Description of the processes that have given rise to the current distribution of initial temperatures and properties in the area in question.

Constituents of the model

Geometric framework
The base for the geometric framework consists of the lithological model and geological-structural model that are set up within the discipline of geology, as well as the hydrogeological model that is developed within hydrogeology. With reference to the investigations conducted on the intact rock, the geometric model can be further subdivided to get volume units with similar properties.

Parameters
Initial temperature conditions.

Thermal properties such as thermal conductivity, heat capacity and coefficient of thermal expansion.

Data representation
A uniform distribution of data is striven for within the volume in question. For the most part, however, constant parameter values are associated with selected objects in the rock volume. Statistical distributions are sought after for representation.

Boundary conditions
Initial temperature conditions and heat flow.

Numerical tools
RVS is used for interpretation and presentation of the constructed model. Numerical calculation models are used to simulate the processes that have created the present-day distribution of temperature.

Calculation results
Distribution of properties in accordance with the above parameter list plus distribution and magnitude of initial temperature within the area.

2 Strategy for estimating thermal properties

2.1 Identification of input data and interaction with other disciplines

2.1.1 Overview of required data and interaction with other disciplines

Identification of input data is an essential part of the thermal modelling strategy. Input data are summarised in Table 2-1. Input data comprise:

- Models produced in other disciplines and aspects of the overall site descriptive model.
- Primary data from measurements of thermal properties.
- Primary data from other measurements in the rock mass.

The site descriptive model consists of models produced in a number of disciplines. These models are developed jointly and iteratively. The geological model and in minor extent the hydrogeological model contain valuable information for the development of the thermal model. Especially the geometrical framework and rock type description/distribution is of interest. Thermal properties and parameters are summarized in Table 1-1.

/Andersson 2003/ describes a strategy for integrated evaluation of the site descriptive models. In /SKB 2002/ the interaction is described between site modelling, repository engineering (design) and safety evaluation.

2.1.2 Geological and geometrical description

The geological modelling is briefly described in /SKB 2001/ and further outlined by /Munier et al. 2003/. The geological models include the geological evaluation and are essential to the understanding of a site. The deformation zone model also includes the geometry of regional and local major and local minor deformation zones. The rock domain model describes geometry and spatial distribution of predominant rock types.

Table 2-1. Models and primary data used as input to the thermal model.

Type of data	Source	Description
Geological description	Geological site descriptive model	Geological evolution (including tectonic evolution), rock domain and spatial distribution of rock types and of fracture zones, characterisation of fractures zones, statistics on mineralogical distribution in rock types.
Hydrogeological description	Hydrogeological site descriptive model	Distribution of hydraulic conductivity, groundwater flow and pressure, that may influence the thermal behaviour.
Geophysical properties of rock	Core and borehole logging. Surface measurements	Fracture, porosity, density and temperature distributions measured along drill cores and boreholes. Gravimetrical and radioactive surface measurements.
Thermal properties of intact rock and fractures	Measurements	Laboratory and field test on core and surface samples and if possible on fractures. Measurements and estimations of the thermal function of fracture zones and high porosity areas.
Surface conditions	Climatic data	Temperature and climate at the ground surface (over time).
International experiences	Collection of experiences	Experiences in the form of methods and data (thermal properties, heat flow, heat generation etc) of similar types of rock.

The rock mass contains discontinuities in a wide size range, from micro-cracks to regional deformation zones. From a thermal point of view the micro-cracks are included in the intact rock and determined as porosity at laboratory investigations. Single, non-water bearing fractures have none or small effects on the thermal properties. Fracture zones of different sizes can have a“convective” or an “insulation” effect on the heat flow depending on if they are water bearing or not.

In the geological model, deformation zones are subdivided dependent on the size (length). The model only describes deformation zones greater than 1 km (local minor deformation zones). Zones with a length less than 1 km are only described statistically for each rock domain. The statistical description of the fractures typically comprises:

- Orientation.
- Spatial distribution.
- Size distribution.
- Volumetric fracture intensity.

The statistical fracture parameters may be used to evaluate the thermal properties (mainly thermal conductivity) for non-intact rock. However, the main concern is concentrated to the thermal properties of intact rock.

The geological model is described geometrically by using the concepts of rock types, rock units and rock domains. A rock unit is a volume judged to have a reasonably statistically homogeneous distribution of lithology (rock types) and fracturing statistics. It may contain several different rock types judged to be similar. A rock unit may also contain small-scale inclusions of very different rock types. Each rock unit is defined by its location and is described in terms of rock type distribution and fracture statistics. In addition, several rock units, e.g. those just separated by different fractures zones, may have similar properties. This information is also handled by logical connections in the geological model, where several rock units are assembled into *rock domains*. A rock domain is a region of the rock mass for which the properties can be considered essentially the same in a statistical sense, see also /Munier et al. 2003/.

In the thermal modelling, properties are modelled for the different rock domains. Of practical reasons, mainly for simplifying the stochastic simulations, different rock types with similar properties are put together in Thermal Rock Classes (TRCs); see Section 3.3.4.

2.1.3 Hydrogeological description

The hydrogeological description contains information on the hydraulic conductivity distribution in the rock mass. In the model, hydraulic properties of the different rock units in the geological model are characterised. Information is given on mass flow in water bearing zones. This information may be essential for the thermal model when the non-intact rock should be described from a thermal point of view. A hydraulic structure in the rock mass causes convective heat transport. Since the thermal properties of the intact rock, at some distance from major water bearing structures, is of greatest importance, the thermal properties of fractured intact rock has not been given priority.

2.1.4 Rock mechanic description

The elevated temperature in a repository influences the stress distribution due to thermal expansion of the rock. The strategy for a rock mechanics site descriptive model is outlined in /Andersson et al. 2002/. /Hökmark et al. 2006/ have made calculations of thermoelastic stress for the KBS-3 repository.

2.1.5 Geophysical properties

Geophysical properties such as density and porosity are determined from direct measurements on core samples and from borehole loggings. Density and porosity of core samples will be determined using standards /SKB 2001/. The initial and natural temperature distribution in the rock mass and the geothermal gradient along water-filled boreholes are measured by temperature logging.

Rock characterisation of individual cores is essential for the interpretation of the borehole loggings of temperature, density and porosity. Density and porosity loggings should be used to describe the spatial distribution of thermal properties in the rock mass. Section 2.3.5 describes how density loggings of boreholes can be used to determine thermal conductivity. Rock characterisation is also used for describing the samples selected for laboratory measurements of thermal properties.

The internal heat production within the rock mass is determined from laboratory or surface testing of Radioactive content (Uranium, Thorium and Potassium).

2.1.6 Thermal properties

Thermal properties are measured on samples in the laboratory, in situ in the rock mass or are calculated from the mineral content. The laboratory method uses core samples from intact rock. The in situ measurements can be carried out with direct methods or indirect methods. The direct methods include multi-probe measurements on outcrops and single probe methods or thermal response tests in drilled boreholes. An indirect method is logging of density followed by calculation using a known relation between thermal properties and the density of the rock; see Section 2.3.5.

2.1.7 Surface conditions

Temperature and other climatic data at the ground surface are received from local weather measurement stations (Swedish Meteorological and Hydrological Institute).

2.1.8 International experiences

International experiences can be received from the continuous use of conventional methods or the development of new methods. Experiences may also exist from data collections from similar rock types.

2.2 Influence on thermal transport properties

The totally dominating thermal transport process in crystalline rock is thermal conduction. Forced convection or convection by gravitation may occur only in hydraulic structures. The thermal transport due to forced convection is normally small due to the low flow of water in the rock mass.

The thermal conductivity of crystalline rock is mainly influenced by the following factors:

- Mineral composition.
- Temperature.
- Fluid/gas in micro-fissures.
- Anisotropy and heterogeneity.

2.2.1 Mineral content

Variations in the mineral distribution for a rock type results in differences in the thermal conductivity. Quartz has 3–4 times higher thermal conductivity than most other minerals. Thus, the quartz content normally has a great influence on the total thermal conductivity. However, for rock types with low quartz content other minerals have a dominating effect.

Assuming isotropic and homogeneous conditions, the thermal conductivity can be calculated from the mineral composition. This is described in Section 2.3.4.

The thermal conductivity of some minerals, for example plagioclase, depends on the chemical composition of the mineral. The chemical composition is often largely unknown and is therefore an uncertainty factor. Compared to thermal conductivity, the heat capacity of different minerals has a lower variation.

2.2.2 Temperature

Studies of the temperature dependence of the thermal conductivity of common rocks presented in literature have shown a decrease in thermal conductivity with the temperature. The decrease may be in the order of 5–15% per 100°C /Sibbit et al. 1979/. An increase of the heat capacity with the temperature has been reported in the literature.

Investigations in the Laxemar and Simpevarp areas show that thermal conductivity for the different rock types decreases by between 1 and 5% per 100°C (means for different rock types) increase in temperature /Sundberg et al. 2006/. In the Forsmark area, the thermal conductivity decreases at higher temperatures with an arithmetic mean of 10.0% /100°C temperature increase (varies between 6.2–12.3%) for the dominating rock type granite to granodiorite /Sundberg et al. 2005a/.

Heat capacity exhibits large temperature dependence; on average an increase with 25% per 100°C increase (0.25%/K) for the three dominant rock types investigated in Laxemar and Simpevarp /Sundberg et al. 2006/. In Forsmark, the heat capacity increases at higher temperatures with a mean value of 27.5% /100°C temperature increase (varies between 15.9% and 54.8%) for the dominating rock type /Sundberg et al. 2005a/.

The temperature influence on thermal properties must be included in the thermal modelling. The temperature also has an influence on the density, in the case volumetric capacity needs to be transformed to specific heat capacity.

2.2.3 Porosity and pressure

The porosity of crystalline rock is low, in general less than 1%. Part of the pore space is in the form of micro-fissures. These micro-fissures have a low influence on the thermal conductivity if they are water saturated or if the rock is under pressure. The pressure dependency of thermal conductivity is generally low, provided that the rock is water saturated /Walsh and Decker 1966/.

2.2.4 Anisotropy

In anisotropic rocks, the thermal conductivity is different in different directions; see Figure 2-1. This has to be considered when evaluating heat transfer in anisotropic rock. /Kappelmeyer and Haenel 1974/ suggested the following expression for an optional angle, φ, between two major directions:

$$\lambda = \lambda_x \cdot \cos^2 \varphi + \lambda_y \cdot \sin^2 \varphi \qquad (2\text{-}1)$$

where λ is the combined thermal conductivity of the isotropic rock and λ_x and λ_y is the thermal conductivity in the x and y direction, respectively. The anisotropy factor is defined as the

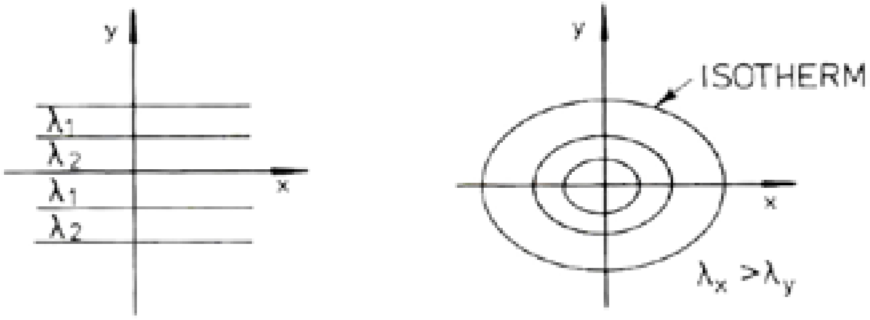

Figure 2-1. *Anisotropy /Sundberg 1988/. Thermal conductivity is denoted by λ.*

ratio of thermal conductivity of the high-conductive and low-conductive directions. Thus the anisotropy factor is always ≥ 1 (equal to 1 for an isotropic rock).

The laws of harmonic and arithmetic composition /de Marsily 1986/ may be used to obtain upper and lower bounds of the thermal conductivity of anisotropic rock.

There are two main types of thermal anisotropy to consider:

1. Anisotropy due to foliation/lineation.
2. Anisotropy due to orientation of rock bodies.

The first type is a structural anisotropy caused by foliation and lineation which occur within a rock type. The foliation and lineation imply a directional orientation of the minerals in the rock mass. The thermal conductivity is generally higher parallel with the mineral foliation and lower perpendicular to the foliation plane. This is because conductive minerals will control the heat flow parallel to the foliation; the minerals extend longer in this plane and are not interrupted to the same extent by less conductive minerals. Perpendicular to the foliation there is a higher density of transitions between different minerals, resulting in less conductive minerals having greater influence. This is accentuated by the crystallographic orientation of the commonly occurring minerals in a rock, such as quartz and biotite.

In addition, a visually isotropic rock may exhibit anisotropic thermal properties due to the orientation of the minerals. The reason is that there may be anisotropy in the minerals due to the properties of the crystals. For example, biotite and quartz have significant different thermal conductivity in different directions of the crystals. Thus, the rock may be anisotropic if the minerals for some reason are oriented in preferential directions, although this is not visually obvious as foliation/lineation. Of course, this type of anisotropy could be present also when there is foliation/lineation.

The second type of anisotropy is a result of the spatial orientation of magmatic rock bodies, primarily subordinate rocks. These bodies may have preferential directions in space, resulting in anisotropy of the thermal properties. Amphibolites parallel to the foliation at Forsmark are typical examples of this anisotropy /SKB 2005/.

In addition to these types of anisotropy there are also other types that could occur, at least theoretically. Anisotropy may be caused by heterogeneity within a rock type, i.e. by different spatial trends in the composition of a rock type in different directions.

2.2.5 Heterogeneity

Heterogeneity in thermal properties is an effect of the lithology in combination with heterogeneous mineral composition of individual rock types. The difference between the two concepts of anisotropy and heterogeneity is illustrated in Figure 2-2.

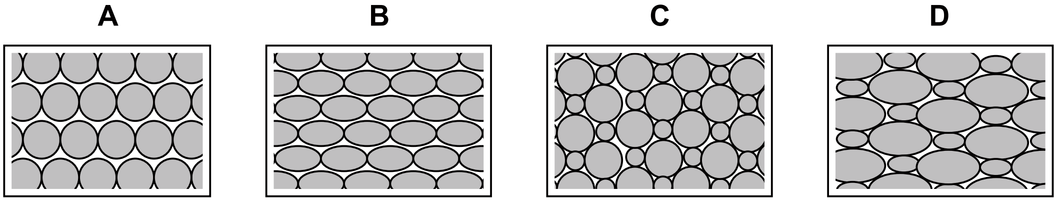

Figure 2-2. The concepts of heterogeneity and anisotropy: A) homogeneous isotropic material, B) homogeneous anisotropic material, C) heterogeneous isotropic material, and D) heterogeneous anisotropic material /Norrman 2004/.

2.3 Determination of thermal transport properties

2.3.1 Introduction

In addition to regular laboratory investigations, thermal properties can be determined using other methods:

- Field measurements of thermal properties.
- Modelling from mineralogical composition and distribution.
- Modelling from density logging.
- Modelling from temperature logging.
- Correlation to rock type from geological description.

A special case is the thermal properties of rock close to, and within, fracture zones. The properties for these types of elements are difficult to measure in laboratory.

2.3.2 Laboratory measurements

There are different types of laboratory methods to determine thermal properties; see for example /Sundberg 1988/. The recommended method for the site investigations is the TPS (transient plane source) method /SKB 2001/. The TPS method is described in /Gustafsson 1991/.

The method is primarily to be performed on drill core samples. The samples are rather small with a diameter of less than 100 mm and a length of approximately 100 mm. The penetration into the sample depends on the size of the measurement probe; with standard probes approximately 10 mm to 14 mm /Sundberg et al. 2005c/.

The TPS method has been used in different investigations at Äspö HRL /Sundberg and Gabrielsson 1999, Sundberg 2002/. The method has been compared with the divided bar method used for the Finnish site investigations. The comparison was made for 17 samples and showed satisfactorily agreement regarding the mean values for all samples but rather large individual discrepancies /Sundberg et al. 2003/.

The TPS-method also allows for measurement of thermal anisotropic conditions. However, such an evaluation demands that the sample is orientated due to the principal axes of the anisotropy and that the heat capacity is known and determined separately with an independent method, for example the calorimetric method.

2.3.3 Field measurements

The principle in situ methods for measuring thermal properties are thermal probe methods and thermal response tests. The in situ methods usually give a characteristic value for a larger volume compared to laboratory measurements. The field methods can be used as a complement to the laboratory measurements. Modelling based on laboratory measurements involves upscaling from small-scale data, a procedure associated with uncertainties, in particular regarding the size of the variance reduction of thermal conductivity. Measurements of thermal conductivity at scales that are significant for the canisters are important in order to minimise these uncertainties. The most relevant scale for investigating variations in thermal properties in a rock volume is not fixed but is governed by the temperature modelling method used in the design of a final repository. In practice, the metre scale is considered to be the most relevant, since at this scale, small-scale variations have been evened out and a considerable reduction in variance can be expected.

A review of different field methods are made in /Sundberg 2006/ in order to propose suitable methods for measurement in relevant scale.

Thermal probe methods

A review of different probe methods can be found in /Sundberg 1988/. A heat-generating probe with a temperature gauge is inserted into the rock. Thermal properties are evaluated from the relationship between temperature increase and time. A variant of the method is the multi-probe method, first described by /Landström et al. 1979/. The multi-probe method makes it possible to evaluate thermal properties of rock over a larger volume, in different directions and over joints. In situ measurements with this method have been performed at the prototype repository at Äspö HRL /Sundberg and Gabrielsson 1999/. The typical scale for single- or multi-probe measurements is in the range of 0.2–1 m.

The temperature field in the rock mass is influenced by differences in thermal properties in the fracture zones in the rock mass. A fracture zone can have an insulation or conductive/convective influence on the heat flow. The thermal function of a fracture zone is dependent on the thermal transport properties and orientation of the zone in relation to the direction of the heat flow. The thermal properties of a fracture zone may be measured by the multi-probe method.

Measurements with the multi-probe method can be performed to analyse the thermal conductivity in different directions in anisotropic rocks. However, this demands simultaneously measurement of the temperature response in two directions, parallel and perpendicular to the anisotropy, and a more advanced evaluation technique.

Posiva has developed a probe for in situ measurements of thermal properties in deep boreholes (TERO-probe). The probe is developed for 56 mm boreholes and the Tero56 device, measurement principle and interpretation techniques is described by /Kukkonen et al. 2005/.

Thermal response test

The method of thermal response tests has been suggested as a potential thermal characterisation method for the site investigations /SKB 2001/. The method can in principle be described as a large-scale probe method (described above) that makes it possible to evaluate a mean value of the thermal conductivity and the thermal diffusivity for the rock mass around a borehole, Figure 2-3. Primarily, an apparent thermal conductivity is determined with this method. The analysis assumes heat transfer through thermal conduction only but the measured actual heat transfer also includes possible convective heat transport. The method is described by /Gehlin 2002/ and has been tested and evaluated at Äspö HRL /Sundberg 2002/. The typical measurement scale for thermal response tests is in the range of 5–100 m.

When the method was evaluated /Sundberg 2002/ the thermal conductivity was estimated from laboratory measurements on core samples along the borehole. In the particular case, the thermal response test was assumed to overestimate the thermal conductivity with about 25%. The reason for this was primarily estimated to be a combination of water movements in (parts of) the borehole due to high-pressure gradients and thermal expansion of the water. The small temperature rise during the test also made the temperature measurements sensitive to different disturbances.

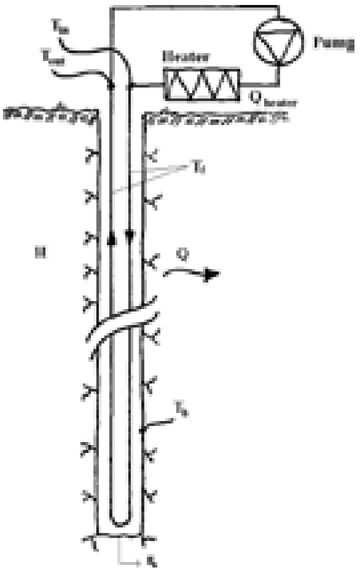

Figure 2-3. *The principle of the thermal response test /Gehlin 1998/.*

The thermal response test may be used for large-scale measurements of the rock mass if the uncertainties described above can be measured and held under control. The method gives a large-scale value of the thermal conductivity. For design purposes it is more interesting to know the distribution of conductivities for blocks at a scale of 1–10 m.

2.3.4 Mineralogical composition

The heat capacity of rock can be computed from volume integrations. The thermal conductivity of composite materials, such as rock, is much more complicated to calculate. In /Sundberg 1988/ an overview of different approaches to the subject is given.

For calculations of thermal conductivity from mineral compositions, the self-consistent approximation (SCA) of a 2-phase material was suggested by /Bruggeman 1935/. For hydraulic conductivity, this has later been redeveloped for n-phase materials /Dagan 1979/. Transformed to thermal conductivity /Sundberg 1988/, the method assumes each grain to be surrounded by a uniform medium with the effective thermal conductivity. In a n-phase material, the effective thermal conductivity, λ_e, can be estimated from the following expression by a number of iterations:

$$\lambda_e = \frac{1}{m}\left[\sum_{i=1}^{n}\frac{v_i}{(m-1)\cdot\lambda_e+\lambda_i}\right]^{-1} \qquad (2\text{-}2)$$

where m is the dimensionality of the problem, λ_i the thermal conductivity of a grain, ν_i the associated volume fraction of the grain and n the number of phases.

For a log-normal distribution the geometric mean is associated with thermal transport in 2 dimensions /Dagan 1979/.

It has earlier been shown that the SCA is in good agreement with measured values /Sundberg 1988/. However, later investigations at Äspö HRL /Sundberg and Gabrielsson 1999, Sundberg 2002, Sundberg et al. 2006/ indicate a tendency for the self-consistent approximation to underestimate the thermal conductivity by about 5–10% for the actual rock types. This may be due to the limitations associated with the point-counting method used, which does not consider fully the presence of alteration products, which in most cases (e.g. sericite and chlorite) have higher thermal conductivity than the parent minerals. There are also uncertainties related to the reference values of thermal conductivity assigned to the different minerals, particularly those that display a range of compositions, e.g. plagioclase and amphibole. The mineral data are mainly based on literature sources.

Chemical and mineralogical composition are determined using the methods ICP, SEM and EDS /SKB 2001/. /Horai 1971, Horai and Simmons 1969/ and /Berman and Brown 1985/ have determined values for the thermal conductivity and heat capacity of different minerals.

2.3.5 Density logging

Density measurements have been used as an indicator to distinguish between Ävrö granite and Äspö diorite at Äspö HRL /Rhén et al. 1997/. A relationship between density and thermal conductivity for all investigated rock types was later observed by /Sundberg 2002/. Based on all available measurements from Äspö HRL empirical relationships between density and thermal conductivity were derived in /Sundberg 2003a/ and are shown in Figure 2-4. More recent data for Ävrö granite have led to a modified relationship (equation) between density and thermal conductivity /Wrafter et al. 2006/. Heat capacity has not been modelled using the relationship presented here. The typical scale for density logging measurements is approximately 0.2 m.

Using the relationship it is possible to calculate the thermal properties from density loggings in boreholes. An example of thermal conductivity versus depth modelled from density logging in aborehole at Äspö HRL is shown in Figure 2-5. However, the relationship is only valid for rock type Ävrö granite, and for the range of densities that were used to derive the equations.

Density logging is a possible method to evaluate the spatial distribution and correlation structure of thermal properties for many rock types because there is a general relationship between density and thermal conductivity /Sundberg et al. 2007/; see Figure 2-6. Homogenous rock types have normally restricted ranges of density and may not show a clear correlation between these parameters. However, the density log may be possible to use in order to create variograms to study the correlation structure for many rock types. Models to treat altered and porous rock based on density would require a great deal of more data which makes the method impractical for these cases.

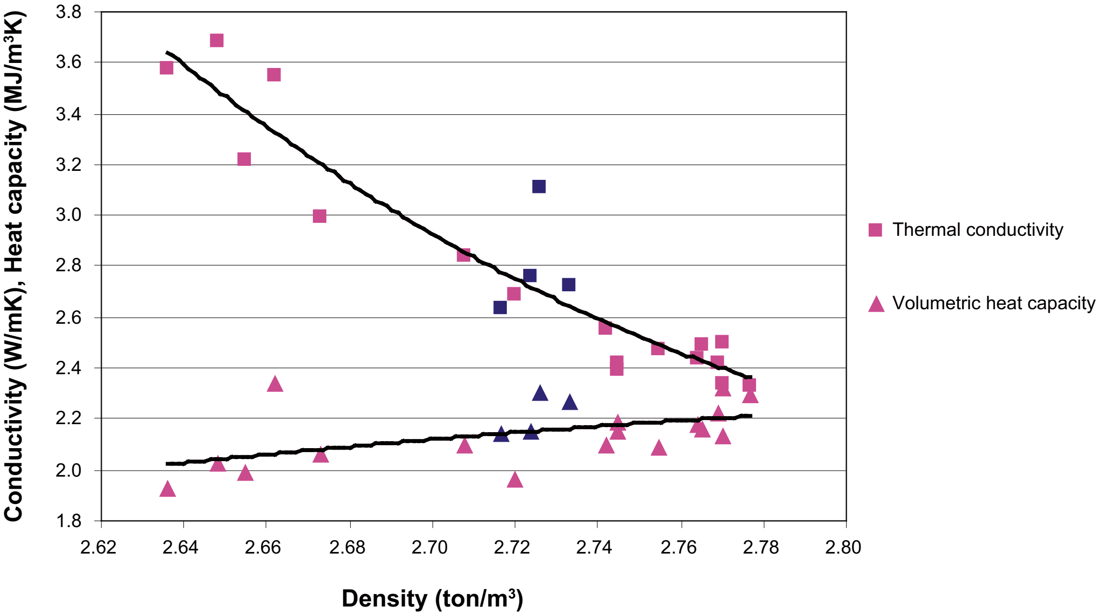

Figure 2-4. *Estimated relationships between density and thermal properties of investigated rock types at Äspö HRL. Values of altered Äspö diorite in blue colour /Sundberg 2003a/.*

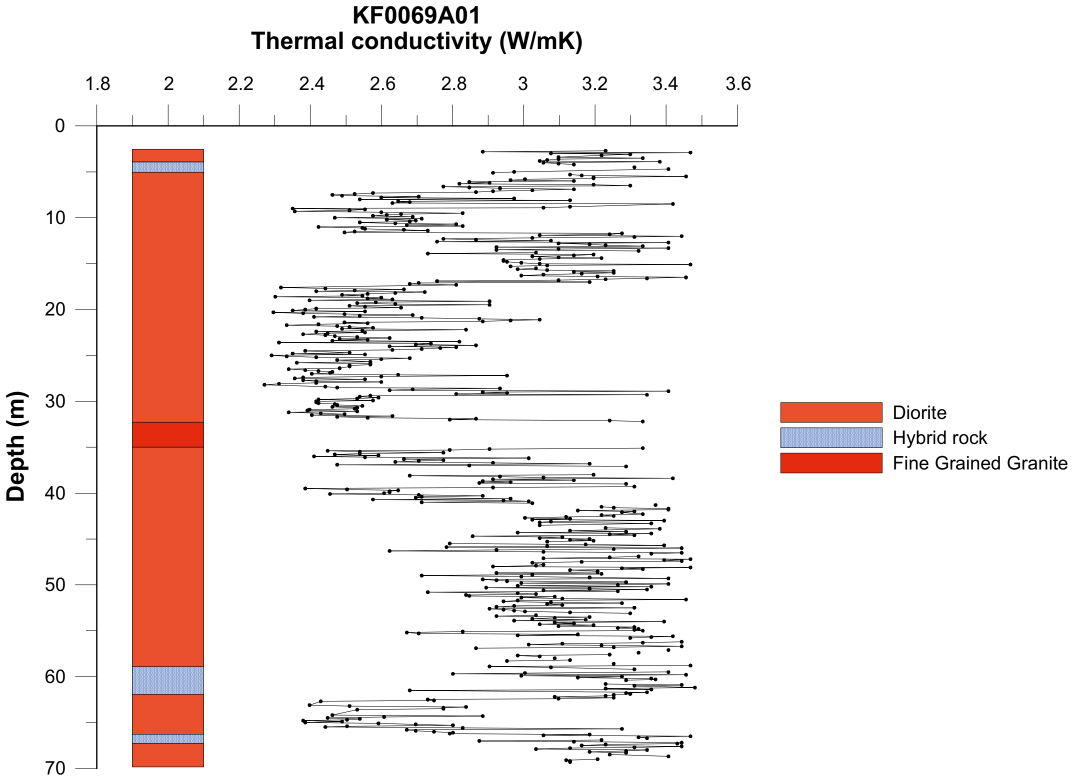

Figure 2-5. *Calculated thermal conductivity (from density logging result) versus depth for borehole KF0069A01 at Äspö HRL.*

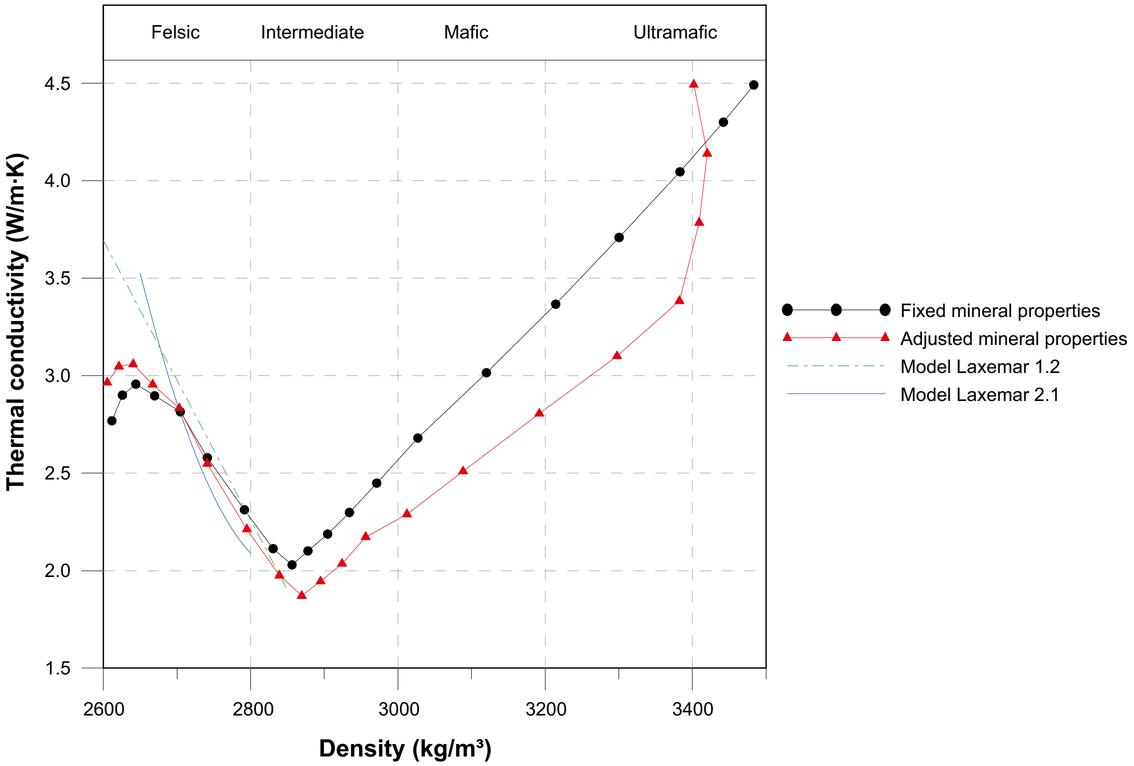

Figure 2-6. *Thermal conductivity vs. density for synthetically defined data with different mineral compositions /Sundberg et al. 2007/.*

It is reasonable to assume that there exists a corresponding relationship between density and heat capacity. Such a relationship can be seen in Figure 2-4, but it is weaker than that for thermal conductivity vs. density. Consequently, a relationship between thermal conductivity and heat capacity could also be expected.

2.3.6 Temperature logging

Temperature loggings can theoretically be used as an indicator of variations in thermal properties along a borehole. However, changes in temperature gradients due to differences in rock type are small, and are in many cases overshadowed by disturbances in the temperature field due to water perturbations or disturbances connected to the drilling. However, the method can be a complement to other methods to estimate the thermal conductivity and at which scale the variations occur. Temperature loggings are also possible to use for evaluation of heat flow data.

2.3.7 Correlation to rock type

Thermal transport properties can be correlated to rock type through the mineral composition (see also 2.3.4). /Sundberg 1988/ made calculations of thermal conductivity from mineralogical composition for about 4,000 samples. Tolerance intervals were created related to rock type. Thus, from the geological description of an area a rough estimation of the thermal conductivity can be made.

2.3.8 Thermal properties of fracture zones

Fracture zones may occur as thermal isolator or conductor dependent on its thermal properties. Depending on orientation, a water-bearing fracture zone may have different functions. If it is orientated perpendicular to the heat flow its thermal function may act as a boundary with constant temperature. If the fracture zone is parallel to the heat flow, its thermal function is a convective additional contribution, or reduction, of the conductive heat transport. When the fracture zone is orientated perpendicular to the heat flow (not water bearing and instead contain clay minerals) it may function as a barrier for the heat flow.

The thermal properties of fracture zones can be evaluated from geological and hydrogeological description and from geophysical data. Theories of calculation of thermal properties of high porosity geological material are involved. However, fracture zones will not be present close to the deposited canisters. The thermal influence on the local temperature field will therefore be quite small.

2.4 Determination of temperature distribution and other thermal data

2.4.1 Temperature logging

Temperature logging in boreholes is used primarily for measuring the temperature distribution in the rock mass and the geothermal gradient. However, there is a clear relationship between temperature, depth, heat flow and thermal properties in the rock mass.

In Sweden, the geothermal gradient is in general about 0.01°C/m, but there are locations with higher values, between 0.01–0.04°C/m, especially in Scania and in mountainous areas with geologically young crystalline rocks /European Commission 2002/. In a report on temperature conditions in the SKB study sites the temperature gradients varies between 0.0095–0.0155°C/m /Ahlbom et al. 1995/.

2.4.2 Internal heat production

The internal heat production in rock can be calculated from the content and radioactive decay of Uranium, Thorium and Potassium. Normally the internal heat production is small and has only a limited effect on the temperature distribution. However, for e.g. young granites the internal heat production may be larger.

2.4.3 Thermal expansion of rock

The thermal linear expansion is measured on core samples in the laboratory. The tests and measurement methods are outlined in SKB site investigation programme /SKB 2001/. Measurements made at Äspö HRL, and as part of the site investigations in Forsmark and Oskarshamn, showed no significant variation due to rock type /Sundberg and Ländell 2002, Sundberg et al. 2005a, 2006/.

2.5 Determination of boundary conditions

2.5.1 Geothermal heat flow

With knowledge of the geothermal gradient and the thermal conductivity of the rock mass it is possible to calculate the geothermal heat flow (see definitions in 1.3.1). A correct heat flow determination requires a correlation between the values of thermal conductivity, the geothermal gradient, changes in temperature conditions at the surface and the particular geology.

The geothermal heat flow is normally 35–70 mW/m². In southern part of central Sweden the heat flow can be somewhat augmented /European Commission 2002/. However, the reliability in such heat flow data can be questioned. The heat flow is seldom measured directly. Instead it is normally calculated from temperature loggings together with assumed, or in same cases measured, thermal conductivities. Uncertainties in the temperature logging result and the thermal conductivity estimation are therefore transferred into the heat flow determination.

2.5.2 Climate conditions at the surface

The actual climate conditions and prognoses for the future can be evaluated from climate databases and from studies by the SKB, for example /Lindell et al. 1999/.

2.6 Data uncertainties

The uncertainties can be divided into the different groups (sections above); see also Section 3.6.

Laboratory measurement

- Performance of the tests and applied test procedures.
- Errors in the methods and limitations of background theories.

Field measurements

- Performance of the tests and applied test procedures.
- Errors in the methods and limitations of background theories.
- Influence of convective transport due to water movements.

Modelling from mineral content

- The accuracy in the modal analyse due to e.g. large grains, alterations of minerals.
- Uncertainties in thermal conductivity of minerals that can have a range of chemical compositions, e.g. plagioclase, amphibole.
- Errors in the methods and limitations of background theories.
- Insufficiencies in thermal data on minerals, especially of the heat capacity.

Density loggings

- The method is restricted to investigated rock types and density interval.
- The empirical relationship contains uncertainties.
- Uncertainties in the density logging determination.

Temperature loggings

- Insufficiencies in the temperature calibration.
- Uncertainties in the temperature determination due to water perturbations in the borehole.
- Borehole temperature may not have achieved equilibrium with the surrounding rock at the time of logging.

Thermal expansion of rock

- Performance of the tests and applied test procedures.

Geothermal heat flow

- Uncertainties in the temperature logging result.
- Uncertainties in the thermal conductivity determination.

3 Site descriptive modelling – assigning thermal conductivity to the rock mass

3.1 Introduction

The strategy for the thermal modelling is to model the spatial statistical structure and perform stochastic simulation to produce a spatial distribution of thermal properties that is representative of the modelled rock domain. The focus is on the most important thermal transport property, thermal conductivity, although heat capacity can also be handled; see Section 3.3.14. Stochastic simulation is used, which is a tool to perform uncertainty analysis or risk analysis. A number of equally probable realisations are produced. These realisations are used to represent the rock domain statistically. There is no prerequisite that data need to be normally (Gaussian) distributed in this strategy. On the contrary, the strategy can handle data from any type of statistical distribution. The methodology implies that no subjective adjustments of the results are required after the simulation phase, as was the case in the previous methodology described in /Sundberg et al. 2005c/. The result will be a more transparent methodology than the approach taken in previous thermal SDMs (up to stage 2.1), and a statistical distribution of thermal conductivity values in a rock domain that better represent the rock mass. The developed methodology based on stochastic simulation is presented in this chapter.

3.2 Expected results

3.2.1 The objectives

The expected results of the thermal modelling can be presented in different ways depending on the objective. According to Section 1.2, the three specific objectives for the thermal modelling methodology are (1) statistical description of the thermal conductivity of a rock domain, (2) prediction of thermal conductivity in a specific rock volume, and (3) visualisation of the spatial distribution of thermal conductivity. The approach to reach these objectives and the expected results are described below.

3.2.2 Description

Of special interest for the objective of description is to:

- determine the low percentiles of thermal conductivity and the associated uncertainty,
- model how the thermal conductivity varies with scale,
- produce realisations of thermal conductivity that can be used for subsequent purposes, such as numerical temperature simulations.

For the description problem, no concern is given to specific locations in the rock mass; only the statistics of the rock domain of interest are addressed, including the uncertainty of statistical parameters. The methodology for this type of problem is based on unconditional stochastic simulation[3]. Expected results are:

- A set of equally probable realisations of thermal conductivity in the rock mass of interest.
- A histogram of simulated thermal conductivity, representing the whole rock mass of interest.

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[3] In principle, conditional stochastic simulation can be used instead but because of the large rock volumes this is not possible for practical reasons (computer limitations). Only small parts of a rock domain can be simulated and therefore unconditional simulation is suggested.

- Statistical parameters of interest, e.g. the mean, variance, standard deviation, percentiles etc.
- Estimates of the uncertainty in statistical parameters, e.g. confidence intervals. This can be used to calculate the probability of encountering low thermal conductivity values below a defined threshold.

3.2.3 Prediction

Prediction of thermal conductivity at specific locations is relevant during for example the construction phase of a repository. Of special interest is to predict the thermal conductivity in the deposition tunnel and around the deposition holes. Prediction requires conditional stochastic simulation, i.e. data from specific spatial locations are honoured during the simulation, in contrast to unconditional simulation. This implies, for example, that simulated rock types will correspond to the rock types that have been confirmed in boreholes, and that simulated thermal conductivity values will correspond to measurements. Expected results are:

- A set of equally probable realisations of thermal conductivity in the rock mass of interest, filling the gaps in the data.
- The most likely thermal conductivity value at a specific location, and a statistical distribution of possible values (uncertainty).
- The probability that the thermal conductivity will be lower than a specified threshold at a specific location.

3.2.4 Visualisation

The visualisation objective is mainly for communication purposes. Visualisation in 3D can be performed for:

- Individual realisations of geology.
- Individual realisations of thermal conductivity.
- Calculated spatial probabilities, such as probabilities that thermal conductivity is lower than a specified threshold.

The 3D visualisations help to understand how thermal conductivity is distributed spatially within a specific rock type, and between rock types.

3.2.5 Application of the results

The result of the site descriptive thermal modelling is a set of equally probable realisations of thermal conductivity. These realisations can, for example, be used for mathematical modelling of temperatures in and around a repository. This can be performed in different time and geometrical scales. The “global” solution contains the large-scale temperature field covering the repository and the surroundings, and includes both short and long-term influence of boundary conditions. The local solution contains the temperature distribution on and around a canister.

The mathematical temperature modelling can be made for the following phases:

- Modelling of the natural temperature distribution
- Modelling of the temperature distribution during construction
- Modelling of medium and long term thermal behaviour

The first point implies a prediction of the natural thermal conditions. However, the natural large scale thermal process is rather insensitive to errors in terms of the determination of the thermal transport properties, the spatial distribution and the boundary conditions. In combination with expected disturbances on the temperature loggings, modelled temperature results may not fully agree with measured temperatures.

The construction may disturb the temperature distribution due to ventilation and machines. However, this influence can be quite difficult to predict and therefore the value of such a modelling can be questioned.

Modelling of the thermal behaviour after deposition of canisters is made in the design and safety assessment. Prediction of the future temperature field is essential for safety assessment and accurate design. The thermal property model must be of sufficient extent so that it can be used for describing the temperature field in both the global and local scale.

3.2.6 Limitations

There are limitations in the methodology concerning the objectives of description, prediction and visualisation. The stochastic simulation does not produce data; it merely fills the data gaps in a structured and logical way while considering the uncertainty. Stochastic simulation is thus not a substitute for lack of data. For example, prediction cannot produce correct values at locations where no measurements have been made. In addition, it must be stressed that there does not exist one single realisation which is the most probable one; instead there is an infinite number of equally probable realisations. However, at a specific location, it is possible to determine the most likely value[4].

3.3 The methodology

3.3.1 Outline

The methodology for thermal modelling is presented in Figure 3-1 and consists of the following steps:

1. Choice of simulation scale
2. Preparation of lithological data (hard data)
3. Defining Thermal Rock Classes (TRCs) within the rock domain
4. Preparation of thermal data (hard data)
5. Change of support
6. Specifying expert knowledge (soft data)
7. Estimating the spatial statistical structure of the TRCs
8. Stochastic simulation of TRCs
9. Estimating spatial statistical thermal model for each TRC
10. Stochastic simulation of thermal conductivity
11. Merging of realisations
12. Upscaling of simulation results
13. Presentation of results

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[4] It is possible to produce a map of the most likely value at every location but this is performed by Kriging, not by stochastic simulation. However, such a map is not a good representation of reality because the variance is reduced significantly in the Kriging process, resulting in a smoothing and smearing effect. In stochastic simulation on the other hand, each realisation retains the spatial variance and therefore models the spatial variability better.

The methodology in Figure 3-1 is applied separately for each rock domain. Starting at the upper part of Figure 3-1, the simulation scale (1) is defined as one of the first steps in the methodology. This scale determines how lithological data (2) should be prepared and if a change of support (5) is required for the thermal data (4). The lithological data acquired from boreholes and mapping of the rock surface need to be reclassified into Thermal Rock Classes, TRCs (3). The main reason is to simplify the simulations; only a limited number of classes can be handled in the simulations for a rock domain.

The lithological data are used to construct models of the transition between different TRCs, thus describing the spatial statistical structure of each TRC (7). The result is a set of transition probability models that are used in the simulation of TRCs (8). The intermediate result of this first stochastic simulation is a number of realisations of the geology, each one equally probable.

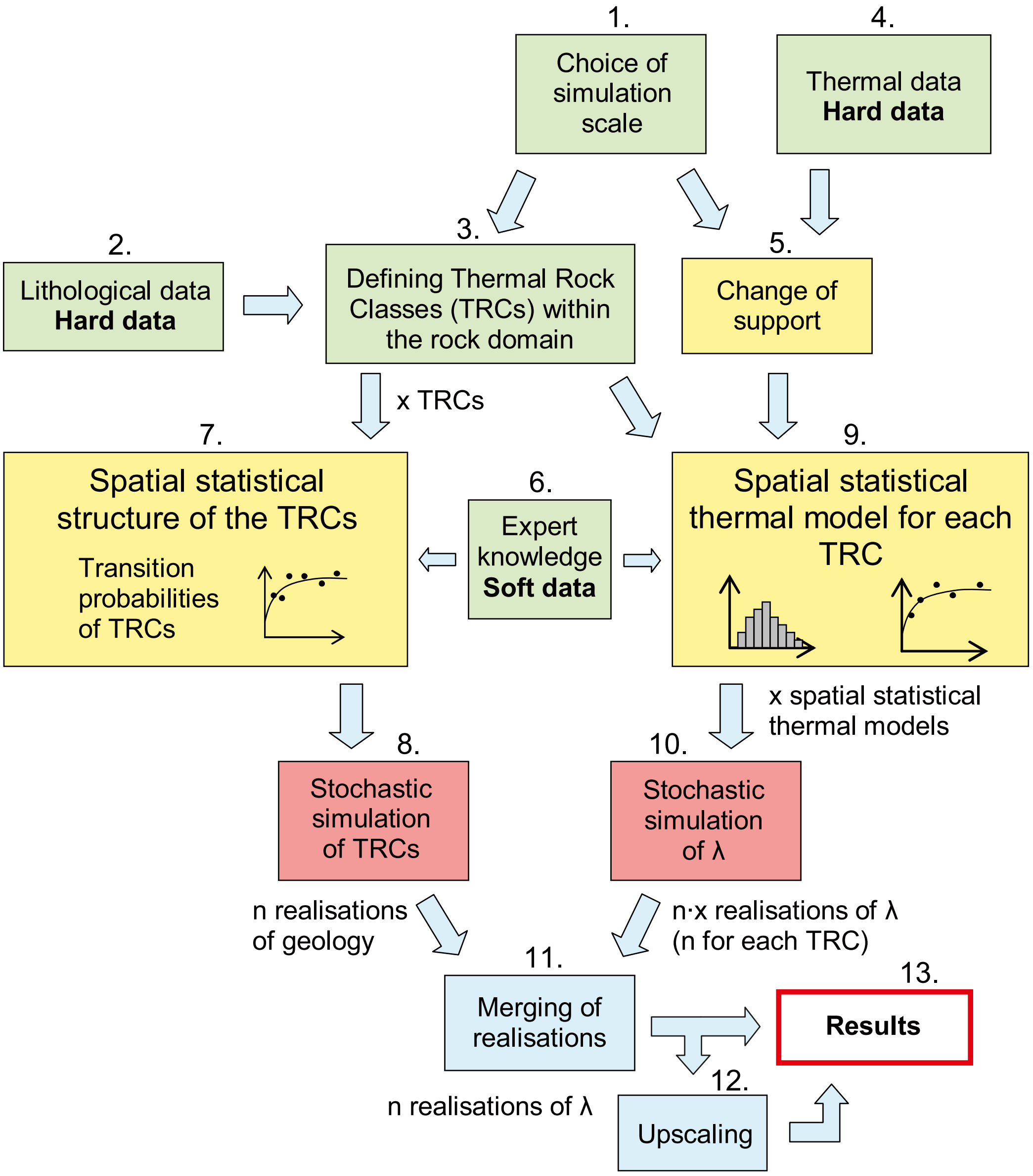

__Figure 3-1.__ Schematic description of the procedure for thermal modelling (λ represents thermal conductivity). The approach is primarily developed for modelling of a rock domain but can also be applied to smaller volumes of rock, if required.

Based on the thermal data, a spatial statistical thermal model is constructed for each TRC (9). It consists of a statistical distribution and a variogram for each TRC. These are used in the stochastic simulation of thermal conductivity (10) and the result is a number of equally probable realisations of thermal conductivity. Steps 9/10 can be carried out in parallel with steps 7/8 because they are independent of each other, provided that the TRCs (step 3) have been defined properly.

In the next step, the realisations of TRCs (geology) and thermal conductivity are merged (11), i.e. each realisation of geology is filled with simulated thermal conductivity values. The result (13) is a set of realisations of thermal conductivity that considers both the difference in thermal properties between different TRCs and the variability within each TRC. If the result is desired in a scale different from the simulation scale, upscaling of the realisations can be performed (12). Upscaling can be performed up to a scale not larger than the size of the simulation domain[5]. The result can be presented in a number of ways, for example as 3D illustrations, histograms and statistical parameters for the rock mass, probabilities of encountering low thermal conductivity data etc.

Graphical illustrations of the outputs from each step are provided in the pilot study in Appendix B.

3.3.2 Choice of simulation scale – step 1

The scale used in the simulations is decided at an early stage. The simulation scale is here defined as the size of a grid cell in the simulation. The simulation domain is defined as all the grid cells in a realisation. Due to practical restrictions, such as computer capacity and time limitations, the practical limit for the number of grid cells is currently in the order of 10^6 in a simulation domain.

The following considerations are taken into account when choosing the simulation scale:

- Preferable, the simulation scale should be equal to the scale (support) of measurements. This will make change of support (Section 3.3.6) unnecessary.
- The simulation scale must be sufficiently small to reflect small-scale variations in lithology and thermal properties that may be of importance. Typical lengths of the important rock types should be considered.
- For 3D simulations representing large rock volumes, the simulation scale must be sufficiently large so that the number of grid cells does not become too large.
- The data requirements in SKB's design work must be considered when the simulation scale is defined.

Some of the issues above are contradicting[6]. It may therefore be necessary to perform thermal simulations in two steps, starting with a small simulation scale; see Figure 3-2. After a change of support, according to Section 3.3.6, a simulation at the larger scale can be performed.

In order to take small-scale rock occurrences into account a simulation scale of 0.1 m is recommended. This scale is sufficiently small to approximately coincide with the measurement scale for thermal laboratory data (TPS method). Change of support is therefore not required for such data.

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[5] In practice, upscaling should be made to a much smaller scale, preferable the canister scale.

[6] For example, the simulation scale should be sufficiently small to reflect small-scale variations but sufficiently large to make possible simulation of large rock volumes, which are two contradicting objectives.

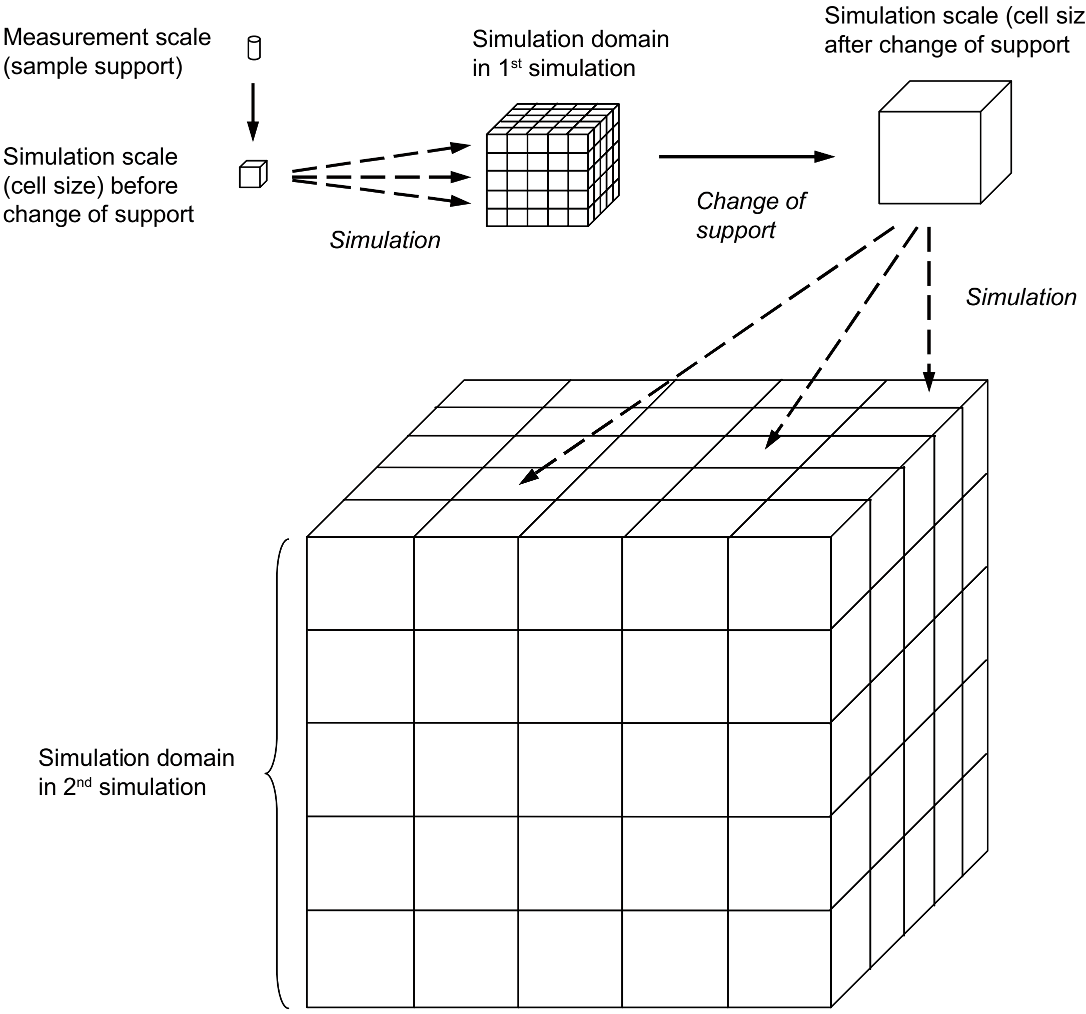

Figure 3-2. *Schematic description of sample support, simulation scale, simulation domain and change of support. A two-step simulation procedure is suggested when change of support is required.*

A simulation scale of 0.1 m implies that the simulation domain is restricted to approximately $10\times10\times10$ m^3 due to practical restrictions. Visualisation of larger rock volumes requires a larger simulation scale. Representing a rock volume of approximately $100\times100\times100$ m^3 can be achieved with a simulation scale of 1 m, i.e. a change of support is required. For visualisation of a whole rock domain, even larger simulation scales are required.

Note that simulation at the 0.1 m scale could be sufficient to statistically represent a rock domain (see “Description“ in Section 3.2). Each realisation will be too small to properly represent the rock domain but all realisations combined may be enough, given that the number of realisations is sufficiently large.

3.3.3 Preparation of lithological data (hard data) – step 2

The lithological information mainly consists of data from cored boreholes, but may also include data from the surface mapping, i.e. outcrops. All drill cores have been mapped to assess the lithology. The disadvantage of the available data from boreholes is that they mainly describe a vertical transect. Horizontal continuity is difficult to assess because only data for separate distant boreholes is available. When applicable, surface data from outcrop mapping can be used. These data are often only available locally in fairly small areas and represent the surface only. The lithological data should be complemented with expert opinion when required (Figure 3-1).

The lithological data needs to be processed before it can be utilised. The resolution in Boremap data is 1 cm, but the resolution in data that will be used in the simulations should match the simulation scale, i.e. the size of a grid cell. Both dominating and subordinate rock types are considered but a problem is how to handle subordinate rock types with an apparent thickness less than the cell size. There are two main approaches:

1. The threshold approach.
2. The probabilistic approach.

In the threshold approach, a threshold is used to determine if the apparent thickness of a rock occurrence in a borehole is sufficiently large to be included in the data set. If the thickness is lower than the threshold, the rock occurrence is omitted. Typically, a threshold of half the cell size is suitable, i.e. a resolution of 0.1 m means that rock occurrences which are less than 0.05 m thick are disregarded. However, for rock types with low thermal conductivity values, a lower threshold could be motivated.

For large data sets, the probabilistic approach is an option. This is best illustrated by an example: Assume that a simulation scale of 1 m is desired. Each 1 m section in a borehole is therefore assigned a rock type that is randomly taken from the 1 m section in the borehole (due to the resolution in Boremap there may be several rock types within that 1 m section but only one of them is randomly selected to represent the whole section). This means that all subordinate rock types are properly represented if the data set is sufficiently large.

How subordinate rock types are considered is especially important for rocks with low conductivity, such as amphibolite. A probabilistic or semi-probabilistic approach, as described, is recommended for such rock types. It is important to remember that using thresholds could result in biased statistics.

The data processing must consider the inclination of boreholes, so that representative statistics of the spatial structure of TRCs can be developed; see Section 3.3.8).

3.3.4 Defining Thermal Rock Classes within the rock domain – step 3

The purpose of this step is to define the Thermal Rock Classes (TRCs) that will be used in the stochastic simulations. The reason that TRCs need to be defined instead of using the rock types directly is that there may be a large number of rock types but only a limited number of classes can be handled in the simulations. By defining TRCs the complexity of the simulations can be kept at a reasonable level. The TRCs implies a rougher classification than rock types but the TRCs are sufficiently detailed to handle the thermal conductivity. It may be required to define separate TRCs for different rock domains because the occurrence of a rock type varies between the rock domains; see Section 2.1.2. It is important to note that TRCs does not mean any reclassification of rock domains[7]; they remain the same, as defined in Section 2.1.2.

The following is taken into consideration when defining TRCs:

- The most important rock types from a thermal point of view are defined as separate TRCs. The importance of a rock type is determined based on (1) how common its occurrence is in the rock domain, and (2) the shape and absolute values of the thermal conductivity distribution. Rock types with low thermal conductivity values are most important.
- Rock types with similar thermal conductivity are grouped into one single TRC, if required. The reasons for combining them are documented. The similarity is assessed based on plotted histograms and calculated statistical parameters.

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[7] The concept of TRC has similarities with the concept of rock domain, although the purpose is different. An important difference is that TRCs are defined for a particular rock domain, without defined spatial boundaries between each class, i.e. a TRC is a categorical variable.

- Rock types with very different spatial variability and correlation should not be grouped in a TRC. These aspects can be assessed by comparing variograms of the rock types.
- Geological aspects, such as composition, age, genesis, mode of occurrence are considered when a TRC is defined. If these aspects differ a lot between two rock types, they should only be combined if the difference in thermal conductivity is insignificant.

A check of the physical properties of the different rock types of a TRC can be performed, e.g. by comparing density values, plotted Streckheisen diagrams etc for tentative compositions of the rock types. Such tests can increase the confidence in the expected thermal conductivity of a TRC.

The defined TRCs can be summarised in a table; see the example in Table 3-1. The code for a TRC is defined by using the two last digits of the rock code for the dominating rock type in that class.

3.3.5 Preparation of thermal data (hard data) – step 4

The different types of thermal conductivity data are presented in detail in Section 2.3. The main data types are:

- TPS (Transient Plain Source) measurement at the laboratory.
- Field measurements at larger scales.
- Calculated values from modal analysis, calculated by the SCA-method (Self-Consistent Approximation).
- Calculated from density logging data.

The data type that is believed to best represent small-scale thermal conductivity is the TPS data. The large-scale thermal conductivity is best represented by field measurements. These two types of data are the main source of information for defining histograms for Thermal Rock Classes (see Section 3.3.10), although SCA data may also be used.

The most important information about spatial variability is believed to be density logging data, i.e. for those rock types where a relationship exists between density and thermal conductivity.

As for lithological data, a data processing step is required also for thermal data. The data processing consists of error checking and, if required, declustering. Checking of errors and low

Table 3-1. Example of defined Thermal Rock Classes (TRCs) for rock domain 029 at Forsmark.

Thermal Rock Class	Rock types	Rock codes
TRC 57	Granite to granodiorite	101057
	Granite, aplitic	101058
TRC 61	Pegmatite	101061
	Granite, fine to medium grained	111058
TRC 51	Granite, granodiorite and tonalite	101051
	Felsic to intermediate volcanic rock	103076
	Tonalite to granodiorite	101054
	Granodiorite	101056
TRC 17	Amphibolite	102017
	Diorite	101033

representativeness in data are required because of human errors but more important because of the difficulty in classifying rock samples of varying composition and alteration into defined rock classes. Outliers in the data set are good indicators of such problems.

If data are spatially grouped in clusters, it may be necessary to use a technique to assign different weights to the data values, giving lower weight to data in clusters. This technique is called *declustering* and is described in detail by /Isaaks and Srivastava 1989/. The reason for performing declustering is to reduce potential bias in the statistics due to the clustered data. Declustering is especially important to perform if the rock sample locations are biased towards high-conductive or low-conductive parts of the rock mass.

The requirements of thermal data are:

- It is desirable that the thermal data represent the same volume as the grid cells in the simulation, i.e. the sample support is the same as the simulation scale. If this is not the case a change of support is required; see Section 3.3.6.
- It is desirable that the amount of thermal data is enough to produce reliable histograms and variograms for each TRC. If this is not the case, expert knowledge will be required as a complement; see Section 3.3.7.

3.3.6 Change of support – step 5

The support of a measurement is the volume, shape and orientation that the data value represents /Starks 1986/. A change of support (upscaling) is required when the support is significantly smaller than the simulation scale, i.e. smaller than the grid cells in the simulation domain; see Figure 3-2. In addition, a change of support may be required when different types of data should be combined, such as laboratory measurements and field measurements representing different scales.

Change of support results in a changed shape of the histogram; the variance is reduced and the mean is slightly affected. However, change of support is a source of uncertainty and should therefore be avoided if possible. The best way to avoid the support problem is to use data that have the same support as the volume we intend to estimate, in our case the simulation scale /Isaaks and Srivastava 1989/.

If a change of support is required, the recommendation is to use stochastic simulation as a tool to perform the upscaling. Thus, the two-step simulation procedure illustrated in Figure 3-2 is applied for each TRC. The principle is simple:

1. Perform 3D simulation at a simulation scale that is close to the scale of the measurements.
2. Divide the simulation domain into cubes of the size of the desired larger scale[8].
3. Take the thermal conductivity values of all grid cells in a cube and calculate the effective thermal conductivity for the cube, using the self consistent approximation (SCA) method[9]. Repeat this for all cubes.
4. Estimate the spatial statistical thermal model of the upscaled thermal conductivity according to Section 3.3.10 and perform stochastic simulation (Section 3.3.11).

The spatial statistical thermal model for the new support (scale) is derived by fitting a distribution model and a variogram model to the calculated histogram and variogram, respectively.

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[8] In Figure 3-2, the desired scale corresponds to the simulation domain and consequently there is only one cube after change of support.

[9] The theoretical framework for the change of support is summarised in Appendix A. Equation A-2 is applied for the upscaling and the effective thermal conductivity λ_e is calculated by iteration.

3.3.7 Specifying expert knowledge (soft data) – step 6

In cases when hard data discussed in Sections 3.3.3 and 3.3.5 are not sufficient, expert knowledge will be required as a complement in order to complete the spatial statistical structure of TRCs and the spatial statistical thermal models; see Section 3.3.8 and Section 3.3.10 respectively. Existing hard data from boreholes and observations at the ground surface provides important but partial knowledge of the geological conditions in a rock domain. The spatial statistical structure of TRCs can be much improved and more realistic with the inclusion of geological expert knowledge. In cases where hard data are restricted to borehole observations, expert judgements, such as geological interpretations of typical geometries of rock types, their orientation and mutual relations and correlation structure, are necessary inputs. Expert knowledge is also required when the lithology in different boreholes belonging to the same rock domain is statistically different (an indication of statistical heterogeneity). Geological expert knowledge must be used to assess the representativeness of the different boreholes and if/how the domain should be divided into more statistically homogeneous subdomains.

The spatial statistical thermal models (statistical distribution and variogram) requires expert knowledge concerning the reasonable shape of histograms and the proper values for variogram parameters, especially if data are sparse or biased for the TRC of interest. Expert knowledge is also required to describe the correlation structure in the three spatial directions, especially in the two horizontal directions where data are sparse when input data mainly originate from vertical boreholes.

Expert knowledge will also be needed when different thermal data sets for one TRC have significant different statistics, such as different histograms and variograms. The main reasons for such differences are lack of representativeness of data (systematic error) and random errors in data. Differences in measurement scale (support) or different measurement techniques can also contribute to dissimilarities. A typical example of these problems is the different histograms of TPS data and calculated thermal conductivity data (SCA) for the same rock type; see /Sundberg et al. 2006/.

3.3.8 Estimating the spatial statistical structure of TRCs – step 7

Prior to simulation of the TRCs, the spatial statistical structure of the different TRCs has to be modelled. Traditionally, in spatial statistical analysis for geological applications the following approach is used:

1. Calculate values of a spatial statistic (usually the semivariogram) at regularly-spaced lags (separation vectors).
2. Fit a mathematical function (e.g. spherical, exponential) through the variogram measurements.
3. Implement various estimation (e.g. Kriging) or simulation (e.g. sequential simulation, simulated annealing) procedures.

Geological or “subjective” knowledge does not necessarily enter directly into this procedure. Another approach to model spatial conditions in geological systems is by Markov chain analysis, where the transitional trends between geological materials are analysed. Spatial modelling using Markov chain analysis makes it possible to more directly and explicitly consider factors with geological meanings, such as:

- volumetric proportions of rock categories,
- mean lengths, e.g. mean thickness in the vertical direction,
- juxtapositional tendencies, i.e. how one categorical variable tends to locate in space relative to another,
- directions of anisotropy,
- spatial variations of the above.

Because of the importance of fully acknowledging both hard and soft geological information for the modelling of TRCs, the Markov chain analysis approach is recommended here. Markov methods have previously been used for predictions in the Swedish nuclear waste repository programme; see e.g. /Rosén and Gustafson 1995ab, 1996, Norberg et al. 2002/.

The modelling consists of calculating transition probabilities followed by expert adjustments based on geological interpretations; see Section 3.3.7. Hard data input consists of Boremap data reclassified as TRCs. The resolution in input data should be the same as the simulation scale.

/Carle and Fogg 1997/ describe how transition probabilities can be used to model the spatial structure, using Markov chains. An example is illustrated in Figure 3-3. The probability of a transition from one TRC to another is described in each of the 16 graphs. The example illustrates four different TRCs, i.e. there are 16 different possible transitions. One such transition is from class A to class A, i.e. the TRC is the same when we move one grid cell in the strike direction (left graph in upper row). Another such transition is from class A to class B (second left graph in upper row) and from class B to class A (left graph in second upper row). The probability of a transition from one TRC to another is represented on the y-axis in each graph and the distance between two points is represented on the x-axis.

The transition probability example in Figure 3-3 is for one-dimensional (1D) simulation in the x-direction. For 3D simulations, similar sets of graphs are required also for the y- and z-directions. This results in a total of 3×16 = 48 transition probability graphs when four TRCs are present. Five TRCs requires a total of 75 graphs for 3D simulations.

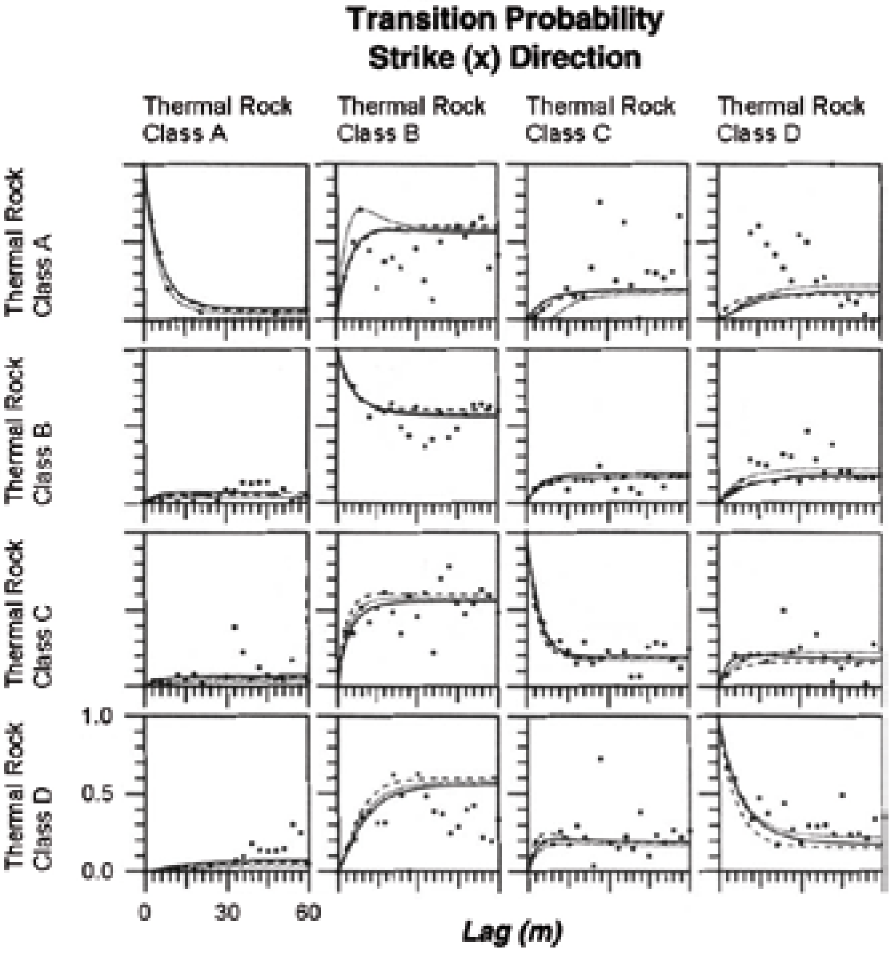

***Figure 3-3.** Principle of transition probabilities using Markov chains for 1D simulation /after Carle and Fogg 1997/. The graphs present the probability of transition from one thermal rock class to another when moving from one cell to the next in the strike direction.*

In practice, software is required for creating the transition probability plots in Figure 3-3. One such software is T-PROGS (Transition PRObability GeoStatistics) /Carle 1999, GMS 2006/. This software utilizes a transition probability-based geostatistical approach to:

1. model spatial variability of categorical data, such as TRCs, by 3D Markov Chains,
2. set up indicator Co-Kriging equations for predicting rock categories at positions where observations have not been made, and
3. formulate the objective function for simulated annealing for finding the global maximum of the prediction model, i.e. for finding the optimal spatial configuration given the selected input parameters.

More information on how the transition probabilities are calculated is given in Appendix B.

Statistical homogeneity is assumed throughout the modelling volume, which is a central assumption in geostatistics. Incorrectly assuming statistical homogeneity of the geology[10] may lead to problems of reproducing the true heterogeneity of the rock domain. Therefore, statistical heterogeneity[11] requires special attention. A solution is to divide the rock domain into subdomains, so that each subdomain can be assumed to be statistically homogeneous. The spatial statistical structure of TRCs is then modelled separately for each subdomain and stochastic simulation of the geology (Section 3.3.9) is also performed separately for each subdomain. The combined realisations of all subdomains are then used to represent the whole rock domain, consideration being taken of the relative volumetric proportion of each subdomain.

An option to Markov Chains is to use indicator simulation. In this case, a set of indicator variograms is calculated instead of transitions probabilities. More information on this approach is given by e.g. /Deutsch and Journel 1998/.

Anisotropy in the lithology requires special attention. For example, it may be necessary to use a local coordinate system with axes oriented parallel and perpendicular to the principal axes of anisotropy.

3.3.9 Stochastic simulation of TRCs – step 8

Simulation of the TRCs, i.e. the spatial distribution of rock types, is performed using categorical variables. Each TRC is identified by a corresponding categorical variable. A set of equally probable realisations of the lithology is built by stochastic simulation. Different simulation algorithms are possible, e.g. Markov chain simulation algorithms /Carle and Fogg 1997/, Markov random fields /Norberg et al. 2002/, or indicator simulation algorithms /Deutsch and Journel 1998/. The suggested method for the simulations is the modified Markov chain method presented by /Carle and Fogg 1997/ for 3D simulations. The commercially available software T-PROGS could be used for these simulations. The software utilizes transition probabilities based on both Markov chains and indicator simulation to create 3D realisations.

First, a model is built of the spatial statistical structure of the TRCs according to Section 3.3.8. Then, stochastic simulation is performed to reproduce the spatial pattern of TRCs. The proportions of the material categories (TRCs) calculated in the Markov chain analysis is kept stationary in all realisations. The result is a set of equally probable realisations of the lithology.

The number of realisations must be decided based on the objective of the simulation and the size of the simulation domain. An example of a 2D-realisation is illustrated in Figure 3-4.

The result of the stochastic simulation must be evaluated. The work can proceed to the next step only if the results (the realisations) are reasonable from a geological perspective. Otherwise,

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[10] The geology is modelled statistically by transition probabilities, according to Figure 3-3.

[11] Typical phenomena that result in statistical heterogeneity are anomalous sizes of rock bodies and anomalous proportions of the various rock types in some boreholes.

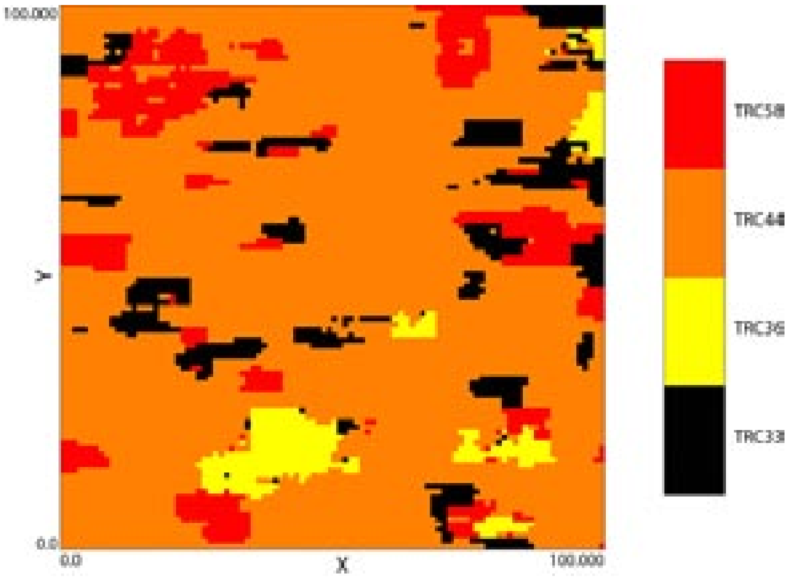

Figure 3-4. *Illustration of a 2D slice from one 3D realisation of TRCs.*

modifications of the spatial statistical structure of TRCs may be required. Revision of the TRCs (Section 3.3.4) may also be needed.

From the realisations it is possible to calculate statistics of the distribution of rock types. Such statistics can include lengths and volumes of rock bodies. Multiple simulations can be required in order to calculate the statistics for various scales.

3.3.10 Estimating spatial statistical thermal model for each TRC – step 9

The spatial statistical thermal model describes the statistics and the spatial correlation structure of thermal conductivity for a TRC. Estimation of the spatial statistical thermal model is performed in three steps for each TRC:

1. Trend analysis.
2. Fitting a distribution model to the histogram.
3. Variogram modelling (structural analysis).

Trend analysis

There may be large spatial trends or statistical heterogeneity in space (non-stationarity[12]) of thermal conductivity for some rock types. A central assumption in geostatistics is the stationarity of the stochastic process. However, the spatial variability heavily depends on the local geology, which is non-stationary in most cases /Brenning 2001/. The assumption that there is statistical homogeneity of thermal conductivity in a TRC, when there in reality is not, may lead to problems of reproducing the true heterogeneity seen in thermal data. Therefore, trends or statistical heterogeneity in thermal conductivity require special attention.

There are usually not enough data to perform a reliable quantitative trend analysis for the whole rock domain but it is suggested that a semi-quantitative or qualitative analysis is performed, e.g. a spatial analysis of the data by graphical plots and by comparing the statistics of different boreholes. If large spatial trends or statistical heterogeneity are detected, it may be justified to model the rock type as two separate TRCs; see Section 3.3.4. Alternatively, the data set of

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[12] See the geostatistical literature for definitions of different types of stationarity, e.g. /Chilés and Delfiner 1999, Journel and Huijbregts 1978/.

a TRC could be subdivided into separate populations and spatial statistical thermal models could be developed for each population (sub-TRC). Stochastic simulations are then performed separately for each sub-TRC. The combined realisations of all sub-TRCs are then used to represent the whole TRC.

Fitting a distribution model

Alternative strategies for this step are:

1. Use the histogram directly, without fitting of a model.
2. Smooth the histogram and use it as a distribution model.
3. Fit a common distribution model (probability density function, PDF) to the data histogram, such as a normal distribution or a lognormal distribution.

The first approach is used when data are believed to properly represent the TRC. Approach two is better when data are sparse. The third approach is only recommended when there is evidence that supports that the thermal conductivity of the TRC follows a common PDF. The smoothing and the fitting of a distribution model require a decision of stationarity to be made. This is a reasonable decision for individual TRCs. A proper decision of stationarity is critical for the representativeness and reliability of the geostatistical tools used /Deutsch and Journel 1998/.

A very important aspect to consider is how to model the tails of the histogram where there are no data. The following principles are suggested for setting lower and upper limits of thermal conductivity in the distribution models for each TRC.

1. The distribution model should cover the range of the data (both TPS and SCA-calculated data).
2. Since the number of data is limited it can be assumed that values outside the range of the data exist. Therefore, it is reasonable to extend the range, depending on the number of data and the appearance/shape of the histogram. This is performed based on statistical principles[13].
3. Where possible, and where justified, a theoretical lower limit (minimum value) can be approximated from assumptions regarding the mineral compositions of “extreme” cases. By “extreme” it is meant mineral compositions which produce the lowest thermal conductivities.

The distribution model of a TRC should reflect all rock types belonging to that TRC. Therefore, it must be taken into account that there are different amounts of data for the different rock types in a TRC. In addition, the percentage of each rock type in the domain will affect the shape of the histogram.

Different types of data are available for some rock types. It may be required to consider data of lower quality than TPS data, such as SCA-calculated data, if data are sparse.

Variogram modelling (structural analysis)

The structural analysis consists in constructing a variogram model which characterises the main features of the spatial variability. This modelling requires good physical knowledge of the thermal properties as well as good “craft” in the practice of fitting geostatistical models /Journel and Huijbregts 1978/. Calculated experimental variograms, covariance plots, madograms and other types of plots of spatial correlation are used in the analysis. Then, variogram models are fitted to the experimental variogram.

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[13] One approach is to base the minimum and maximum values of the histogram on calculated confidence intervals of low and high percentiles, e.g. the 1-percentile and the 99-percentile.

The variogram modelling is a very important step in the thermal modelling because it will dictate how the variance is reduced when the scale increases. This is important for the tails of the thermal conductivity distribution at different scales. The variogram model is associated with modelling uncertainty, which is an important uncertainty to consider in the strategy.

A set of principles are suggested for the variogram modelling:

1. Base the variogram model on the dominating rock type in each TRC.
2. Base the nugget of the variogram on the most reliable data, usually TPS data. Use a low value when the nugget is uncertain; a high nugget may underestimate the lower tail of the thermal conductivity distribution after upscaling.
3. Base the range (correlation length) on density logging data, if possible. Use a high[14] estimate if the range is uncertain; a low range may underestimate the lower tail of the thermal conductivity distribution after upscaling.
4. Use omni-directional variogram models, if data does not suggest otherwise, i.e. calculated down-hole variograms are used to represent all directions.
5. In cases where different types of variogram models exhibit good fit to data, an approach is suggested that does not underestimate the lower tail of the thermal conductivity distribution (conservative approach[15]).

There will be large uncertainties in the variogram modelling for TRCs where data are sparse. Expert knowledge is required as a complement to hard data. Actions to ensure that the lower tail of the thermal conductivity distribution is not underestimated, as described above, are thus recommended.

For some rock types, complex spatial patterns can be expected; see for example the step-wise increase in variance as a function of distance for Ävrö granite in /Sundberg et al. 2006/. Complex spatial patterns can be modelled by so called nested variogram models /Journel and Huijbregts 1978/. Basically, a nested variogram is constructed by adding two or more variogram models. Complex variograms could also be a result of statistical heterogeneity of thermal conductivity within a TRC and between boreholes. Such problems cannot be solved by nested variograms (see the section above about trend analysis for suggestions).

A special type of anisotropy can be handled by variograms, i.e. anisotropy due to heterogeneity within a rock type caused by spatial trends in the composition; see Section 3.4). However, this type of anisotropy is not believed to be significant and a single omni-directional variogram model, representing all three principal directions, is therefore used.

3.3.11 Stochastic simulation of thermal conductivity – step 10

Sequential Gaussian Simulation (SGS) is used for simulating the thermal conductivity within each TRC. Consequently, one simulation is performed for each TRC. The basis for the SGS is the distribution model and the variogram model (Section 3.3.10). The result of the simulation is a set of equally probable realisations.

SGS is a simulation algorithm that performs simulation based on a standard normal distribution[16]. Thermal conductivity follows other statistical distributions. However, this is of limited practical importance because simulation software are designed to perform normal score

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[14] The variability in a single realisation might be underestimated if the range is long compared to the size of the simulation domain. However, this is compensated for by creating multiple realisations.

[15] From this perspective, the Gaussian model is more conservative than the spherical model, which in turn is more conservative than the exponential model. The slower the increase in variance, the more likely it is that low values occur in clusters, which affects the lower tail of the distribution after upscaling.

[16] A standard normal distribution has a mean of 0 and a standard deviation of 1.

transformation of thermal conductivity values before the simulation, and back-transformation of the Gaussian values to thermal conductivity after the simulation. This is performed regardless of the shape of the thermal conductivity distribution. Therefore, normal score transformation and back-transformation is not further discussed.

An important aspect to consider in the simulation is the reproduction of discontinuities, if such exist. A continuous random function model cannot reproduce discontinuities, as found when crossing a physical boundary such as that of a lithotype /Deutsch and Journel 1998/. Examples of such features are deformation zones, water-bearing fractures, dykes of subordinate rock types, portions of altered rock etc. Such features should preferably be handled in the stochastic simulation of TRCs. However, if there is a slow transition from, for example, fresh rock to altered rock it may be better to handle this problem in the stochastic thermal simulation.

It is suggested that one thermal realisation is created for each realisation of lithology (TRCs). Another approach that could be used during initial testing is to perform a number of thermal simulations for only one realisation of lithology. The results from such simulations could be used to study the variability of thermal conductivity within TRCs and compare it with the variability in lithology.

The number of realisations must be decided based on the objective of the simulation and the size of the simulation domain. Because the lower tail of the thermal conductivity distribution is of concern, the number of realisations must be sufficiently large to stabilise the lower tail.

3.3.12 Merging of realisations – step 11

The realisations of TRCs (the geology) and thermal conductivity are merged so that thermal values from each TRC are assigned to a position in space determined by the realisation of geology. Thus, a geological realisation works as a mask for the thermal realisations. The principle is illustrated in Figure 3-5 for 2D-realisations. The result of the merging is one set of realisations of thermal conductivity. These realisations consider both variability due to different TRCs (lithology) and variability within each TRC. All realisations are equally probable.

3.3.13 Upscaling of simulation results – step 12

Upscaling of the simulation results is performed if results are desired for a different scale than the simulation scale. Such upscaling can also be used to study how the result varies with the scale, plotted on a graph. This could be imperative when viewing the rock domain from different perspectives: small scale, canister scale, and repository scale. The upscaling is performed with the SCA approach described in Appendix A. Equation A-2 is applied and the effective thermal conductivity λ_e is calculated by iteration.

3.3.14 Presentation of results – step 13

The main result of the thermal modelling is a set of equally likely realisations of thermal conductivity. How the result is presented will depend on the objective of the simulations; see Section 3.2. For the objective of *description*, the results are presented as:

- A histogram of simulated thermal conductivity, representing the whole rock mass of interest. Of special interest is the lower tail of the histogram.
- Statistical parameters, such as the mean and the 1-percentile (the latter representing the lower 1% of thermal conductivity values).
- Estimates of the uncertainty in statistical parameters, e.g. confidence intervals of the mean and the 1-percentile.
- The probability of encountering thermal conductivity values lower than a defined threshold.

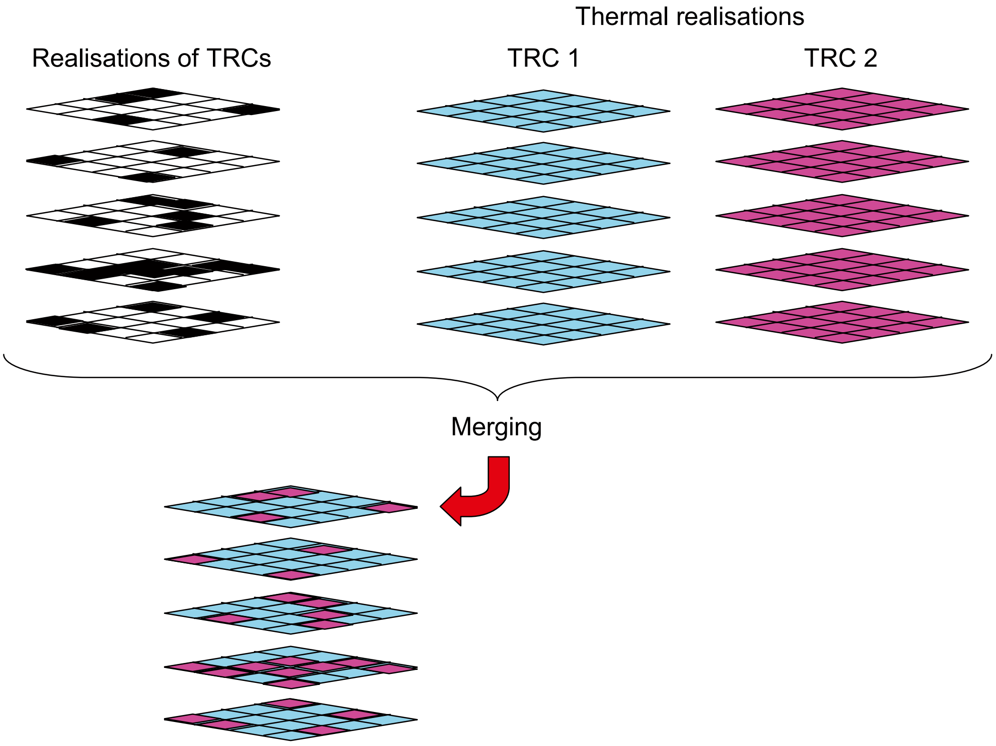

Figure 3-5. *Schematic description of the merging of TRC realisations (geology) and thermal realisations for two TRCs (2D realisations). The geological realisations controls from which TRC a thermal conductivity value is selected. The same principle applies also to 3D-realisations and when there are additional TRCs. The spatial variability of thermal conductivity within each TRC is not illustrated in the figure.*

Examples of results for the objective of *prediction* are: The most likely thermal conductivity value at a specific location, and a statistical distribution of possible values (uncertainty). This means that, for example, it is possible to estimate the probability that the thermal conductivity will be lower than a specified threshold at a specific location.

The main results for the objective of *visualisation* are visualisation of individual realisations of lithology and thermal conductivity. Visualisation of probabilities is also possible, e.g. the spatial distribution of the probability of thermal conductivity below a specified threshold.

In addition, the realisations of thermal conductivity could be used for description, prediction and visualisation of related thermal properties, most importantly heat capacity. As indicated in Section 2.3.5, it can be assumed that there is a relationship between thermal conductivity and heat capacity. By applying this relationship, realisations of heat capacity can be created from the thermal conductivity realisations.

3.4 Handling of anisotropy

The thermal properties of the rock mass may vary in the principal directions of the coordinate system, i.e. there may be different thermal transport properties in the x-, y- and z-directions. According to Section 2.2.4, the two main types of thermal anisotropy to consider are:

1. Anisotropy due to foliation/lineation.
2. Anisotropy due to orientation of rock bodies.

The importance of the various types of anisotropy should be analysed. A significant anisotropy due to foliation/lineation (type 1 above) has been indicated by field- and laboratory measurements. Data from these measurements should be considered when evaluating the simulation results. From the field and laboratory measurements a characteristic value for the anisotropic thermal conductivity can be assessed for each domain, e.g. quantified as an anisotropy factor; see Section 2.2.4.

The anisotropy due to orientation of rock bodies (type 2 above) is handled when the spatial statistical structure of the TRCs is modelled, according to Section 3.3.8. This type of anisotropy can also be quantified by an anisotropy factor. Previously performed calculations indicate that the importance of this type of anisotropy usually is rather small.

In addition to these types of anisotropy there are also other types that could occur, at least theoretically. Anisotropy may be caused by heterogeneity within a rock type, i.e. by different spatial trends in the composition of a rock type in different directions. This anisotropy could be evaluated by directional variograms of thermal conductivity within a TRC, i.e. separate variograms for the three principal directions. This would require large data sets for each direction but because data in the horizontal directions are sparse, this approach is unrealistic at present. However, there is no reason to believe that this anisotropy is significant compared to the other two types of anisotropy. Therefore, this type of anisotropy is omitted in the modelling and down-hole variograms are used to represent all three spatial directions (Section 3.3.10).

The scale of observation must be considered when the thermal properties are evaluated. Changing the scale of observation may or may not have a significant effect on the anisotropy, depending on the type of anisotropy.

If these ways of handling the anisotropy are not sufficient, a more ambitious approach may be required. It is possible to handle the above types of anisotropy in the stochastic simulations, provided that the anisotropy can be properly modelled. A detailed modelling of the anisotropy will require sufficient reliable data and 3D stochastic simulations for each principal direction.

3.5 Special issues in the modelling

There are some issues that may require special attention in the thermal modelling. These include:

- How to model rock types that can be considered as a mixture of two or more rock types with widely differing thermal conductivity irregularly distributed in space (e.g. how to model the rock type Ävrö granite in Oskarshamn).
- How to treat altered rock in the thermal modelling. Altered rock may have significantly different thermal conductivity but data are sparse.
- How to treat fractured rock in the thermal modelling. Fractured rock is not represented in the thermal measurements and density logging data may not be representative.

It is believed that all these issues can be handled within the methodology presented in this chapter. However, simplifications and expert knowledge is required.

3.6 Uncertainties in the modelling approach

A compilation of the uncertainties in thermal modelling is found in /Sundberg et al. 2005c/. Data uncertainties are described in Section 2.6.

Uncertainties of major importance for the strategy in this chapter are:

- Uncertain representativeness of measurements and borehole data. This uncertainty can be handled by alternative statistical models based on subsets of boreholes and measurements. The uncertainty can be reduced by additional representative data.
- Uncertainty in the spatial statistical structure of TRCs. This uncertainty can be handled by performing simulations with alternative representations of transition probabilities.
- Uncertainty in the upscaling methodology. This uncertainty is believed to be small compared to other uncertainties and further improvement has low priority.
- Uncertainty in the statistical distribution models. This uncertainty can be handled by performing simulations with alternative distribution models. It can be reduced by additional data.
- Uncertainty in the variogram models. This uncertainty can be handled by performing simulations with alternative variogram models. The noise in density data can be handled by manipulating the Kriging equations of the stochastic simulation /Dowd 2007/. The uncertainty can be reduced by more thermal data and by further investigation of the relationship between density and thermal conductivity for different rock types.
- Uncertainty due to discretisation (simulation scale) and the size of the simulation domain. The discretisation may result in discretisation errors for subordinate rock types. A small simulation domain may also cause biased statistics, especially after upscaling.
- Uncertainty in the stochastic simulations. All simulation methods have an effect on the output and may introduce their own artefacts /Dowd 2007/. The uncertainty is minimised by using validated simulation algorithms and skilled personnel.

Of these, uncertainties in the spatial statistical structure of TRCs and in the spatial statistical thermal models (distribution models and variogram models) are believed to be the most important for the result, i.e. the model uncertainties. The spatial models are deduced from the relatively sparse data and are then used to generate realisations. Checking that the realisations reproduce the spatial models, e.g. histogram and the variogram, is no guarantee that the model is correct (i.e. we are assuming that the model is known with certainty). This is a very difficult area; see for example /Dowd and Pardo-Igúzquiza 2002/. One way of handling model uncertainty is to apply a range of different models. Stochastic simulation can then be repeated using the different models.

3.7 Validation

Validation of the results of the methodology can be performed at two levels:

1. Validation of the outputs from individual steps in the thermal modelling procedure.
2. Validation of the results of the thermal modelling.

Validation of the steps in the methodology can be performed by comparing the output with true data. For example, histograms of simulation results can be compared against the distribution model, variograms of simulation results can be checked against the variogram model, simulated results can be compared with data by Q-Q plots etc. Examples of these methods are demonstrated in Appendix B.

Validation of the results of the lithological simulations (Section 3.3.9) can be made by performing simulations in rock volumes where the true properties are known, using conditional simulation. The proportion of correctly predicted cells is a measure of the performance. Examples of this approach are demonstrated in Appendix B. Validation of the lithological simulations can also be performed by analysing the statistical distribution of lengths and volumes of rock bodies in stochastic realisations, and comparing them with statistics of field observations and geological expert knowledge.

4 Documentation and quality assurance

4.1 Quality assurance

SKB follows the quality principles as defined in the standard ISO 9001:2000. Technical Auditing (TA) and Quality Assurance (QA) procedures will be applied during the modelling work.

Essential to the quality standard are requirements of adequate documentation throughout the entire modelling work. The key component is “traceability”, of data, processes and results, and of the theories, conceptualisations and assumptions that form the basis for the modelling methods used and the conclusions drawn.

The technical auditing procedures comprise control of the technical content to establish if it is adequate for the purpose. Quality assurance refers to checking that pre-determined procedures are followed and to reviewing non-conforming results. It comprises procedures for control during determination of data and input of data to databases.

Fundamental for quality assurance is that data for modelling are taken from the SKB Site Characterisation Database (SICADA). Firstly, only quality-controlled data may be stored in SICADA, Figure 4-1. Archived information is maintained in accordance with quality assured procedures. Secondly, only data from SICADA may be used for interpretation, analysis and modelling of the investigated sites.

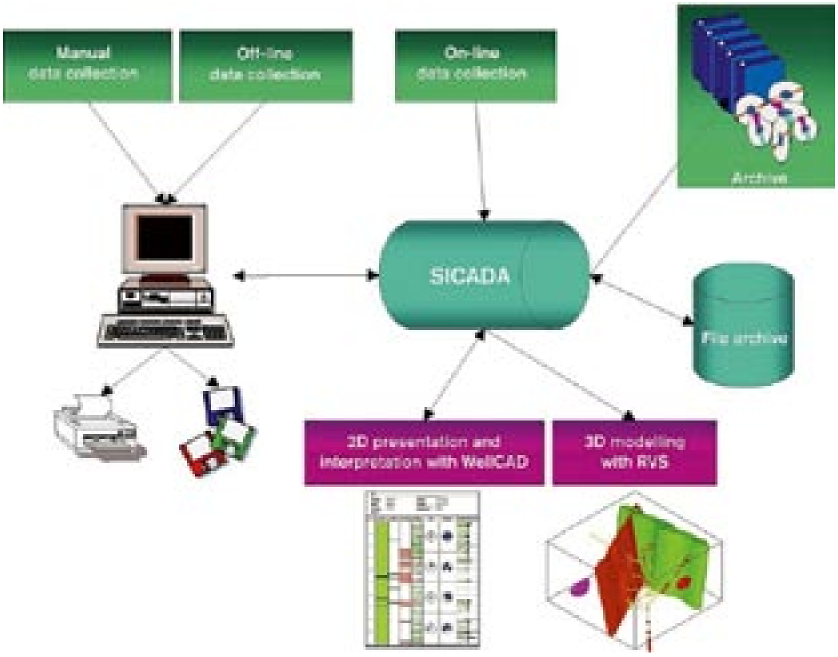

Figure 4-1. *SKB’s database SICADA with associated functions /SKB 2001/.*

4.2 Documentation

A comprehensive report should follow each Thermal Model version. The report should, as a minimum, include the following:

- Input data and supporting models.
- Evaluation of primary input data and input obtained from other disciplines (geology and hydrogeology) of the Site Descriptive Model
- Presentation of the thermal modelling
- A summary description of the modelling results and major uncertainties. The description of uncertainty is an integrated part of the Site Description.
- Recommendations for the next investigation step, if required.

4.3 Continuous improvment of strategy

The presented strategy for thermal site descriptive modelling is a result of technical auditing of the thermal SDMs during the initial site investigation phase at the Forsmark and Oskarshamn areas /Sundberg et al. 2005ab, 2006, Wrafter et al. 2006/; see Section 1.1. The strategy is tested and evaluated for a test case in a pilot study; see Appendix B. In this way technical auditing of the modelling work is rendered possible. The implementation of the strategy for the test case clarifies issues of special importance and difficulty for the description and prediction of thermal conductivity.

If required, the methodology is continuously improved during the forthcoming construction and operation phases.

5 Conclusions

All three specific objectives for the thermal modelling (description, prediction and visualisation; see Section 1.2) are attained with the updated strategy for thermal modelling. The main conclusions are:

- The statistical description of the thermal properties of a rock domain can be performed quantitatively using unconditional stochastic simulation. Almost any type of statistical property can be determined and its associated uncertainty estimated.
- Prediction of thermal properties in a specific rock volume can be performed using conditional stochastic simulation, as illustrated in Appendix B.
- Visualisation of the spatial distribution of thermal properties can be performed for both description and prediction, as illustrated in Appendix B. The visualisation is only restricted by the simulation volumes and software limitations.
- The methodology takes into account the spatial distribution of rock types (lithologies), including statistical properties and Markov properties, and the spatial variability of thermal conductivity within rock types.
- Measurements representing different scales can be handled using the change of support approach (Section 3.3.6).
- Uncertainties are easy to identify and their effect can be estimated, qualitatively or quantitatively. However, the latter may require repeated stochastic simulations.
- The proposed stochastic approach for thermal modelling has a high degree of transparency and flexibility. The mean reasons are the stepwise approach and the combination of lithological and thermal simulations, which allows for site-specific adjustments.
- The presented approach can be applied also for other properties than thermal.
- As a spin-off, the lithological realisations can be used to calculate statistics of the distribution of rock types. Such statistics can include lengths and volumes of rock bodies.

The following aspects should be considered when the strategy is applied:

- The main uncertainties are believed to be uncertainties in the spatial statistical structure of TRCs and in the spatial statistical thermal models. In addition, the choice of simulation scale and associated uncertainties may have a significant impact on the result.
- There exist uncertainties concerning the significant scale (or range of scales) that influences the maximum bentonite temperature. However, these uncertainties can be handled in the following design step.
- Expert knowledge is an important supplement to hard data in the strategy, both for modelling lithology and thermal conductivity.
- The required confidence of the statistical description is higher for the lower tail of the thermal conductivity distribution, especially if the absolute values are relatively low, since this affect the minimum distance between canisters; see e.g. SR-Can /SKB 2006/.
- Accurate description of the lower tail of the thermal conductivity distribution requires a lot of data. For rock types with limited thermal data, the lower tail is uncertain and may even require extrapolation. Therefore, conservative assumptions may be required in order not to overestimate the critical thermal conductivity value for a rock domain.

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Appendix A

Theory of upscaling

Upscaling approaches

/Isaaks and Srivastava 1989/ suggest different methods for transforming one distribution to another, including the affine correction and the indirect lognormal correction. All these methods leave the mean of the distribution unchanged, while the variance is adjusted. However, such transformation methods are sufficient only for quantities that average arithmetically, such as ore grades or pollutant concentrations /Isaaks and Srivastava 1989/. Thermal conductivity, on the other hand, is a transport property (like hydraulic conductivity) and does not average arithmetically. Therefore, other approaches are required. However, it should be noted that thermal conductivity data follow a much more symmetrical distribution than do hydraulic conductivity in rock, which is an advantage. Experience from the site descriptive modelling indicates that thermal conductivity follows a close to normal or slightly lognormal distribution for many rock types /Sundberg et al. 2006/.

Several methods have been developed for change of support related to hydrogeological applications. According to /Gutjahr et al. 1978/ and /Dagan 1979/, the effective hydraulic conductivity depends on whether the problem is 1D or 3D. /Dagan 1979/ presented the following general solution to the effective mean hydraulic conductivity (transformed to thermal conductivity; see /Sundberg et al. 2005/):

$$\lambda_e = -(m-1)\cdot\lambda_x + \left(\int f(\lambda)\, d\lambda / (m-1)\cdot\lambda_x + \lambda\right)^{-1} \qquad \text{(A-1)}$$

where m is the dimensionality (1, 2, or 3) of the problem and f(λ) the frequency function of thermal conductivity λ. If λ_x is replaced by λ_{max} and λ_{min}, the result will be the same as Hashin's and Shtrikman's upper and lower bounds for an isotropic material /Hashin and Shtrikman 1962/. If λ_x is replaced by λ_e, the self-consistent approximation (SCA) is obtained as follows:

$$\lambda_e = 1/m \cdot \left(\int f(\lambda)\, d\lambda / (m-1)\cdot\lambda_e + \lambda\right)^{-1} \qquad \text{(A-2)}$$

For a lognormal distribution, the effective conductivity according to Equation A-2 for two dimensions ($m = 2$) coincides with the geometric mean. For tree dimensions ($m = 3$) the effective conductivity is slightly higher. Equation A-2 is used to calculate the thermal conductivity from modal analysis by iteration /Sundberg 1988/.

If the standard deviation (σ) of the natural logarithms of λ is small, then the effective thermal conductivity can be approximated as follows for a lognormal conductivity distribution /after Gutjahr et al. 1978/:

$$\text{2D: } \lambda_e = \lambda_G \qquad \text{(A-3)}$$

$$\text{3D: } \lambda_e = \lambda_G\,[\,1 + \sigma^2 / 6\,] \qquad \text{(A-4)}$$

where λ_G is the geometric mean thermal conductivity.

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Appendix B

Pilot study of SDM strategy

Introduction

A pilot study of Site Descriptive Modelling (SDM) strategy presented in Chapter 3 was performed on the rock domain Ävrö granite in Laxemar. Real thermal conductivity measurements from the thermal SDM stage 2.1 for Laxemar /Wrafter et al. 2006/ was used but rough assumptions and simplifications were made in order to keep the complexity and required work at a reasonable level for this type of test. Different types of stochastic simulations were performed:

1. Unconditional stochastic simulations of TRCs and thermal conductivity – simulation scale 0.1 m.
2. Unconditional stochastic simulations of TRCs and thermal conductivity – simulation scale 1 m.
3. Conditional stochastic simulations of TRCs in the neighbourhood of borehole KLX06 – simulation scale 0.1 m.

The presentation below follows the step-wise description of the modelling strategy in Chapter 3 and Figure 3-1.

Choice of simulation scale – step 1

The simulation scale 0.1 m (grid cell size 0.1×0.1×0.1 m^3) was used in the first unconditional simulations. This is the same scale as was used in the thermal SDM stage 2.1. After change of support, the simulation scale 1 m was used for the unconditional simulations. The conditional simulations of TRCs around borehole KLX06 were performed with a simulation scale of 0.1 m.

Preparation of lithological data – step 2

Lithological data from five boreholes in Laxemar were used: KLX01, KLX02, KLX03, KLX04 and KLX06. The data consist of Boremap information including rock occurrence of subordinate rock types.

Defining Thermal Rock Classes within the rock domain – step 3

Four Thermal Rock Classes (TRCs) were defined:

TRC 33: Diorite-gabbro (501033) and fine-grained diorite-gabbro (505102)

TRC 36: Quartz monzodiorite (501036) and fine-grained dioritoid (501030)

TRC 44: Ävrö granite (501044)

TRC 58: Granite (501058), fine-grained granite (511058) and pegmatite (501061)

The TRC numbers refer to the two last digits in the rock code of the dominating rock type in each TRC.

Preparation of thermal data – step 4

Only TPS data (laboratory measurements) were used in the pilot study. The data processing was limited, e.g. no error checking was performed. Therefore, the quality of data is not known.

Change of support – step 5

A change of support was performed for each TRC using stochastic simulation and upscaling with the SCA approach. This means that the methodology in Chapter 3 was fist applied at a simulation scale of 0.1 m. After upscaling to 1 m (change of support), the methodology in Chapter 3 was repeated for the 1 m scale. This two-step procedure is illustrated in Figure 3-2.

The histograms of simulation results are illustrated in Figure B-1 for scale 0.1 m and after upscaling to 1 m and 2.5 m. Note that the uncertainty in the histograms increases when the scale is increased. This is because the number of values is reduced due to the upscaling.

The spatial aspect of the upscaling is illustrated in 2D in Figure B-2. The resolution is reduced when the support is increased.

Specifying expert knowledge (soft data) – step 6

Expert knowledge is an important source of information. However, expert assessments were made rough and fast in the pilot study because the aim of the study is to test and illustrate the methodology, not to arrive at high quality results.

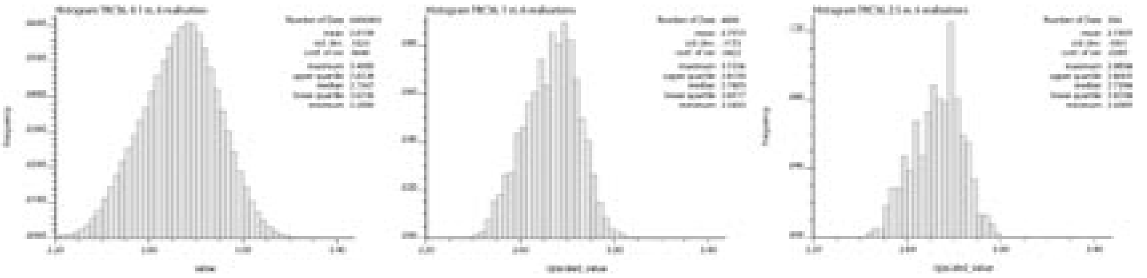

Figure B-1. *Histograms after change of support is performed for a TRC. The support is increased from 0.1 m (left) to 1 m and 2.5 m. The histograms are based on 6 realisations.*

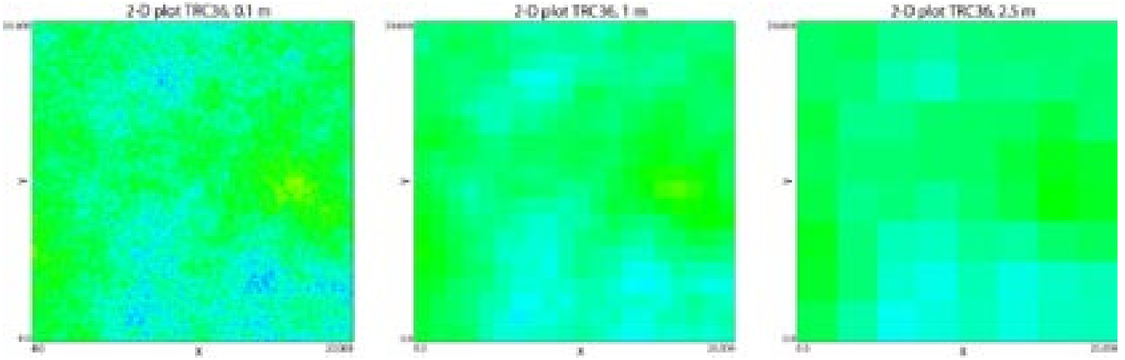

Figure B-2. *One 2D slice from a 3D simulation for one TRC and for three different supports. The support is increased from 0.1 m (left) to 1 m (middle) and 2.5 m (right).*

Estimating the spatial statistical structure of the TRCs – step 7

The software T-PROGS was used for estimating the spatial statistical structure of TRCs and the stochastic simulation of TRCs. T-PROGS facilitates stochastic modelling of lithology based on Markov chain analysis for describing the spatial conditions of lithological categories. The major steps in T-PROGS are:

1. Calculation of transition probability measurements.
2. Modelling spatial variability with Markov chains.
3. Stochastic simulation.

These steps are performed using five different modules; see Figure B-3.

The spatial dependency of material categories are estimated by classical Markov chain analysis. The analysis starts with calculations of the number of transitions between material categories at equally spaced distances (lags). The frequencies are transformed to transition probabilities for the specific lag distance. The probability calculations are displayed in a transition probability matrix, such as:

$$\mathbf{T}\,(\Delta h_z = 1.5\text{ m}) = \begin{bmatrix} t_{11}(\Delta h_z) & \cdots & t_{1K}(\Delta h_z) \\ \vdots & \ddots & \vdots \\ t_{K1}(\Delta h_z) & \cdots & t_{KK}(\Delta h_z) \end{bmatrix} = \begin{bmatrix} 0.63 & 0.11 & 0.0 & 0.04 & 0.22 \\ 0.16 & 0.48 & 0.04 & 0.0 & 0.32 \\ 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.14 & 0 & 0.14 & 0.57 & 0.14 \\ 0.05 & 0.11 & 0.03 & 0.0 & 0.81 \end{bmatrix}$$

Transition probability matrices are calculated for different lag distances. For each transition category, these "experimental" probabilities are plotted against the lag distance. For each transition category, a curve is fitted to the experimental data to model the spatial dependency. Transition probability matrices are estimated for each principal direction in the modelling volume to facilitate three dimensional modelling of spatial dependency; see Figure 3-3 in the main report. Anisotropy is accounted for by using different transition probability matrices for different directions.

Most Markov chain analyses in geological applications have been performed in the form of so called embedded analyses /Carle 1999/, in which transition probabilities of occurrences from one discrete occurrence of a category to another, are considered, irrespective of the lag distance. The embedded analysis thus provides the probabilities of what other category to enter when leaving a specific category and does not directly give information about the spatial dependencies of the categories. T-PROGS links the embedded Markov chain analysis to the development of *continuous-lag* (spatially dependent) Markov chain models. The reason this is important is that geologists are more inclined to think and work in the embedded framework /Carle 1999/.

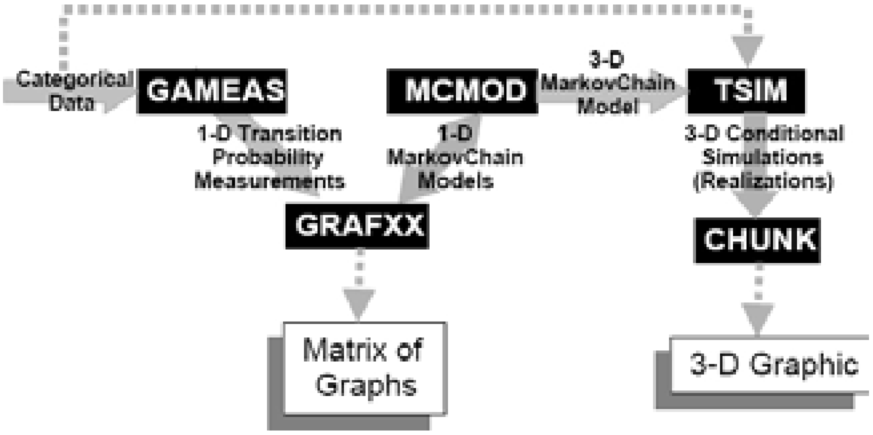

Figure B-3. *The T-PROGS modelling procedure /GMS 2006/.*

Stochastic simulation of TRCs – step 8

An overview of methodology for stochastic simulation of TRCs will be given. For details, the reader is referred to the cited references. Based on the transitional properties analysed by Markov chain analysis, stochastic simulations (conditional or unconditional) of categorical configurations, such as TRCs, are made through a two-step procedure of:

1. Generating an "initial configuration" using a Co-Kriging-based version of the sequential indicator simulation (SIS) algorithm /Deutsch and Journel 1998/ where a transition probability-based indicator co-kriging estimate is used to approximate local conditional probabilities by:

   $$\Pr\{k \text{ occurs at } \mathbf{x}_0 \mid i_j(\mathbf{x}_\alpha);\ \alpha = 1, \ldots, N;\ j = 1, \ldots, K\} \approx \sum_{\alpha=1}^{N} \sum_{j=1}^{K} i_j(\mathbf{x}_\alpha) w_{jk,\alpha}$$

   where N is the number of data, K is the number of categories, $w_{jk,\alpha}$ represent a weighting coefficient, and $i_j(x_\alpha)$ represents the value of an indicator variable:

   $$i_j(x_\alpha) \left\{ \begin{array}{l} 1 \textit{ if category } j \textit{ occurs at } x_\alpha \\ 0 \textit{ otherwise} \end{array} \right. , \qquad j = 1, \ldots, K$$

   Use of Co-Kriging instead of the traditional indicator Kriging approach improves consideration of spatial cross-correlations.

2. Iteratively improving the conditional simulation in terms of matching simulated and modelled transition probabilities by applying the simulated quenching (zero-temperature annealing) algorithm:

   $$\min \left\{ \sum_{l=1}^{M} \sum_{j=1}^{K} \sum_{k=1}^{K} [t_{jk}(h_l)_{MEAS} - t_{jk}(h_l)_{MOD}]^2 \right\}$$

   where O denotes an objective function, the h_l denote $l = 1,\ldots,M$ specified lag vectors, and $MEAS$ and MOD distinguish measured and simulated (measured from the realisation) transition probabilities, respectively /Aarts and Korst 1989, Deutsch and Journel 1998, Deutsch and Cockerham 1994, Carle 1997/. The simulated quenching algorithm is implemented by repeatedly cycling through each nodal location of the conditional simulation and inquiring whether a change to another category will reduce O; if so, the change is accepted. This iterative improvement procedure continues until O is minimized, or a limit on the number of iterations is reached. Conditioning is maintained by not allowing changes of categories at conditioning locations. "Artifact discontinuities" /Deutsch and Cockerham 1994/ are avoided by generation of the initial configuration and including consideration for anisotropy and limiting the number of lags in formulation of the objective function /Carle 1997/.

This procedure is used for each equally probable stochastic realisation being performed. T-PROGS can produce up to 999 realisations in one batch of simulation.

T-PROGS was used for both unconditional and conditional simulations in the pilot study. The following simulations were performed:

1. Unconditional simulations with 1 metre scale resolution. Model dimensions were $100 \times 100 \times 100$ m^3, resulting in a model size of 10^6 cells. Spatial dependency was modelled from boreholes KLX01, KLX02, KLX03, KLX04, and KLX06. A geological anisotropy factor of 2 was applied in the E-W (X) direction of the model. The anisotropy factor was subjectively estimated from the geological map of the area.

2. Unconditional simulations with 0.1 scale resolution. Model dimensions were 20×10×5 m^3, resulting in a model size of 10^6 cells. Spatial dependency was modelled from boreholes KLX01, KLX02, KLX03, KLX04, and KLX06. An anisotropy factor of 2 was applied in the E-W (X) direction of the model. The anisotropy factor was subjectively estimated from the geological map of the area.
3. Conditional simulation adjacent to borehole KLX06 with 1 metre scale resolution. Model dimensions were 80×50×20 m^3, resulting in a model size of 80,000 cells. Isotropic conditions were assumed.

The simulations were visualised using the T-PROGS/GMS interface which facilitates views of the modelled volume from different angles and cross-sections along the principal axes (Easting = X, Northing = Y, and Vertical = Z) of the volume. Figure B-4 shows examples of unconditional realisations at the 0.1 metre scale.

Figure B-5 shows examples of unconditional realisations at the 1 metre scale.

Figure B-6 shows an example of the conditional simulation at borehole KLX06.

Conditional simulation facilitates validation of the model. A simple validation was made by omitting data from the borehole, running the simulations, and evaluating the proportion of correctly predicted positions (cells) along the borehole.

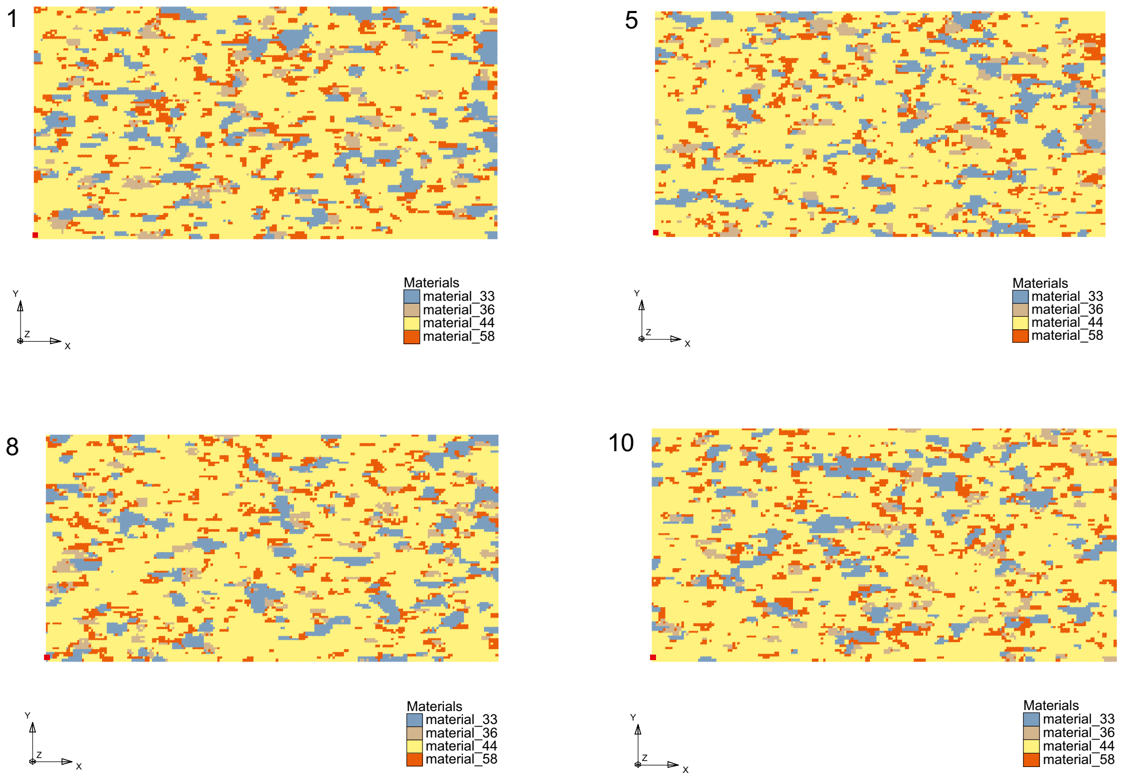

Figure B-4. Examples of unconditional realisations in the 0.1 metre scale. Maps show cross-sections along the XY (horizontal) plane. Numbers indicate the number of the realisation (total of 10).

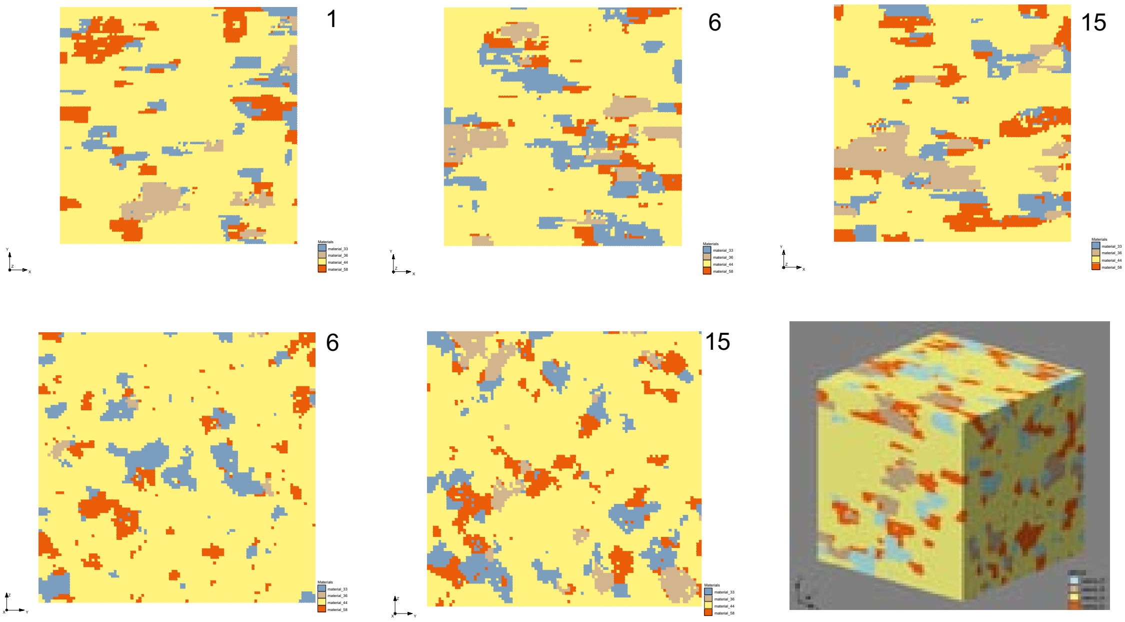

Figure B-5. *Examples of unconditional realisations in the 1 metre scale. Top row shows cross-sections along the XY (horizontal) plane. Bottom row shows cross-sections along the Northing-Vertical (YZ) plane. Anisotropy is in the East (X) direction. Numbers indicate the number of the realisation (total of 25).*

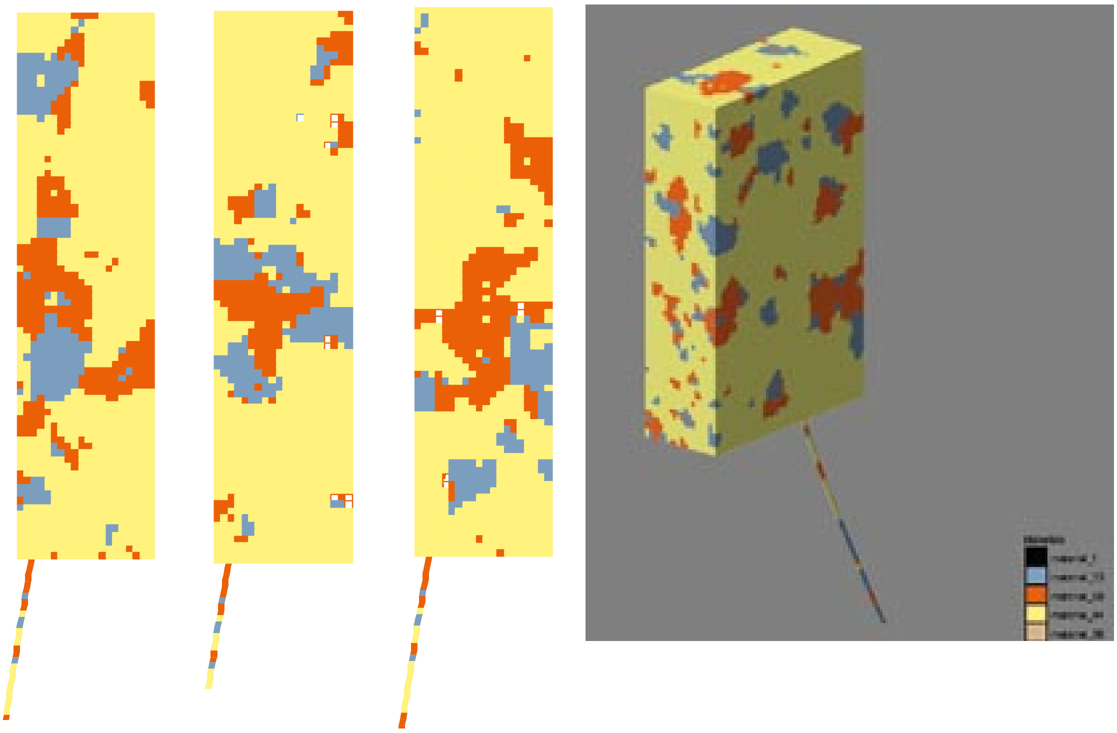

Figure B-6. *Examples of conditional realisations at the 0.1 metre scale around borehole KLX06. Maps show cross-sections along the Northing-Vertical (YZ) plane. The position of the borehole is indicated.*

The validation procedure included the following steps:

1. Markov chain analysis and calculations of the vertical transition probabilities.
2. Assigning the same transition probability matrices to the X and Y directions of the model, thus assuming isotropic conditions.
3. Omitting data from the borehole by randomly selecting positions along the borehole. The following proportions of the borehole information were kept:
   a. 75%
   b. 50%
   c. 25%
   d. 5%
4. Simulation of the model volume for each proportion of kept data. Each simulation consisted of 5 realisations.
5. Calculation of the mean proportion (from the 5 realisations) of correctly predicted cells at positions where borehole data had been omitted.

The results of the validation are shown in Figure B-7.

As expected, the proportions of correctly predicted cells decrease as the proportion of kept data in the borehole decreases. The model is able to give a relatively high proportion of correctly predicted cells (90%) even if the number of kept data in the borehole is as low as 25%. For lower proportions of kept data, the prediction accuracy decreases rapidly. When only 5% of the data were kept in the borehole, the proportion of correctly predicted cells was only 55%. This is approximately the probability of a correct prediction using a total random selection of rock categories, given the proportions (or stationary distribution) of the categories present in the borehole. This indicates that when only 5% of the data is kept, this data is located at positions further apart than the correlation lengths given by the transition probabilities.

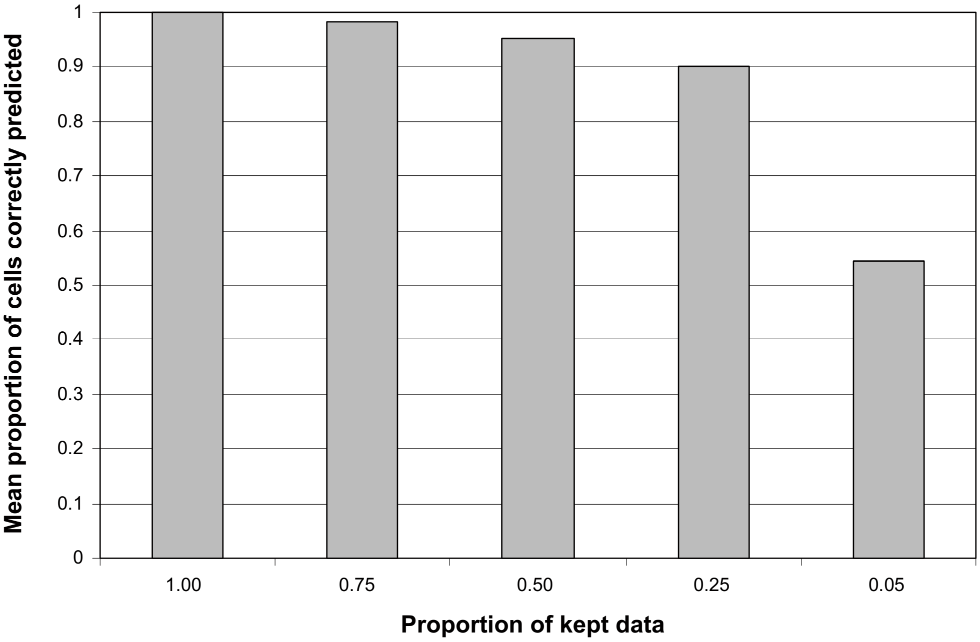

Figure B-7. Proportions of correctly predicted cells along borehole KLX06 vs. the proportion of kept data in the borehole.

Estimating spatial statistical thermal model for each TRC – step 9

Statistical distribution models were defined for each TRC. Figure B-8 illustrates the data histogram for one of the TRCs and the corresponding smoothed model for the 0.1 m scale. A minimum value of 2.20 W/(m·K) and a maximum of 3.40 W/(m·K) was used as limits of the model.

In is good practice to compare the distribution model with the data. The Q-Q plot in Figure B-9 compares the quantiles of data and the distribution model. When the points fall on *any* straight line, the shapes of the two distributions are the same but they may have different means and variances /Deutsch and Journel 1998/. All distribution parameters are the same if the points fall on the line x = y. Figure B-9 indicates that the agreement in distribution shape, mean and variance are fairly good between data and the model, although not identical. Similar plots are can also be made for comparison of cumulative probabilities, so called P-P plots.

Figure B-10 illustrates the corresponding distribution model for the 1 m scale. This histogram is the result of stochastic simulation followed by upscaling from 0.1 m to 1 m.

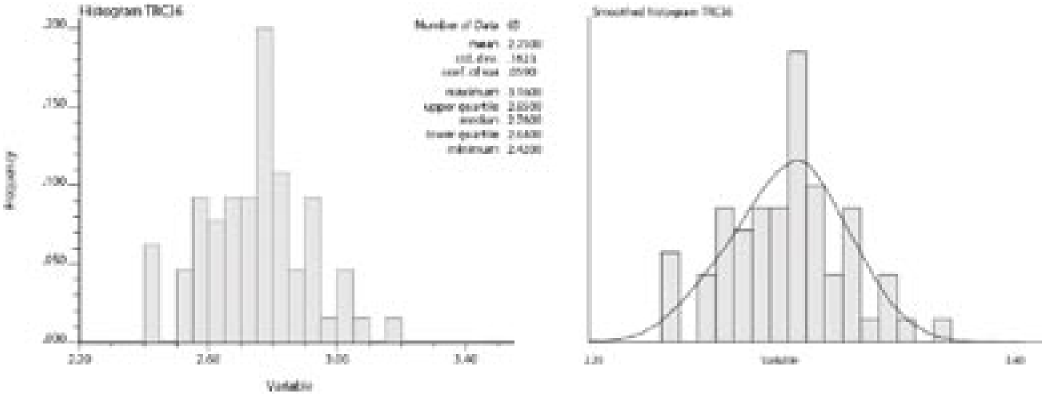

Figure B-8. *Data histogram and distribution model for one TRC (0.1 m scale).*

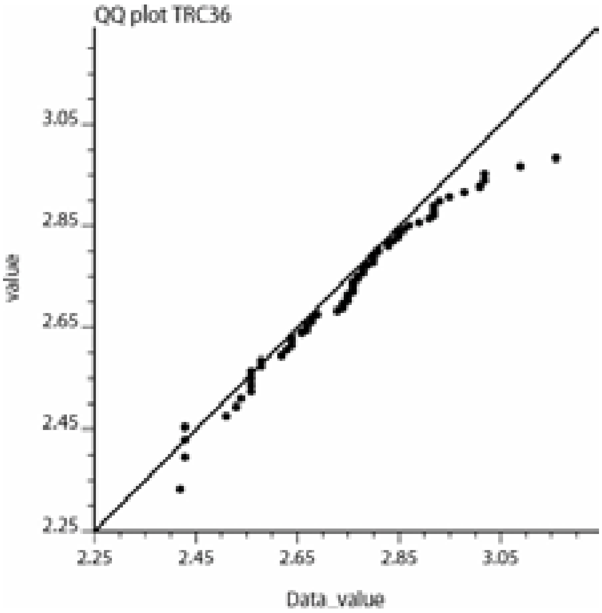

Figure B-9. *Q-Q plot of TPS data (x-axis) versus distribution model (y-axis) for TRC 36.*

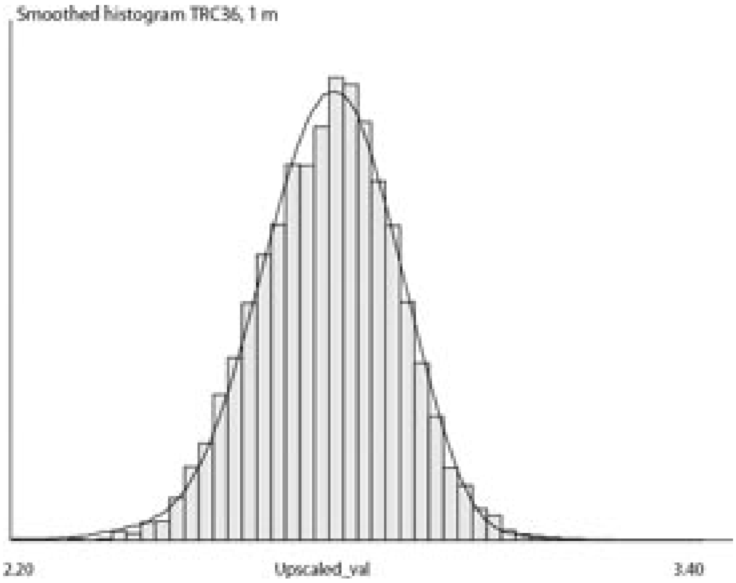

Figure B-10. *Distribution model for one TRC after simulation and upscaling from 0.1 m scale to 1 m scale.*

After normal scores transformation of the TPS data, the spatial correlation was analysed for each TRC. Figure B-11 illustrates a covariance plot and a variogram, including the variogram model (red). The range is estimated from the covariance plot and the nugget from the variogram. Only the two first points of the variogram are reliable due to lack of data. Therefore, the variogram model is highly uncertain. The model could be improved substantially if calculated thermal conductivity values from density loggings were used in combination with TPS data to model the spatial statistical structure. However, this was not performed in this pilot study.

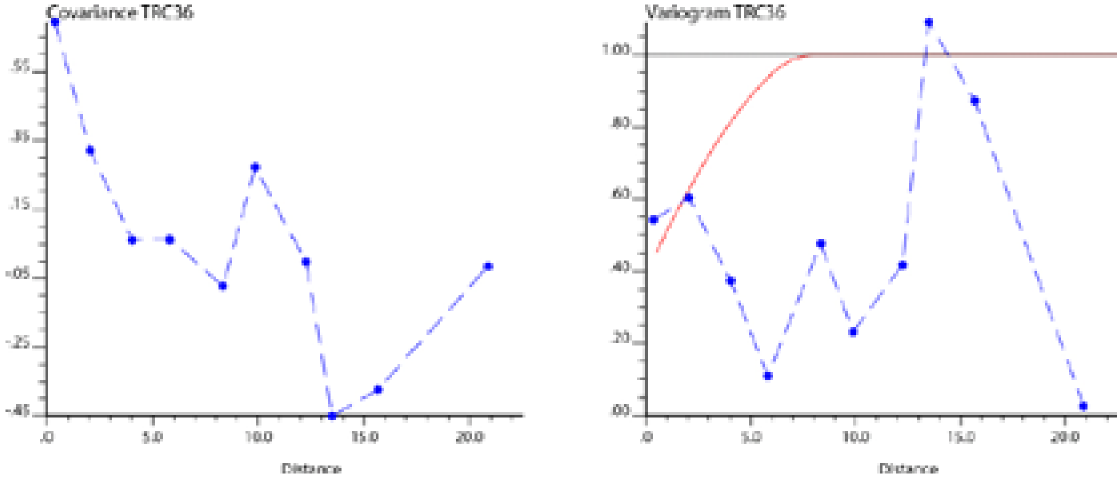

Figure B-11. *Covariance plot (left) and variogram plot (right) for one TRC at the 0.1 m scale based on a limited set of TPS measurements. The range is interpreted from the covariance plot, which is more stable than the variogram. A conservative value of the nugget is derived from the variogram plot (only the two first points in the variogram are reliable due to the limited number of measurements). The resulting variogram model is plotted in red colour (spherical model).*

A different variogram model is required for simulation at the 1 m scale. The nugget of the variogram model is almost eliminated but the range is unaffected. As a rough approximation, the nugget variance is reduced by the ratio of the two support volumes /Dowd 2007/. Upscaling from 0.1 m to 1 m represent a volume ratio of 1,000, i.e. the standardised nugget variance is expected to be reduced from approximately 0.4 in Figure B-11 to 0.0004, which is a negligible nugget.

Stochastic simulation of thermal conductivity – step 10

Stochastic simulation of thermal conductivity was performed using Sequential Gaussian Simulation. This implies that simulated values are drawn from a standard normal (Gaussian) distribution. Simulations were performed independently for the four TRCs based on the developed spatial statistical thermal models. After the simulation, all simulated values were transformed back to thermal conductivity space.

3D-simulations with a simulation scale of 0.1 m was performed in a simulation volume of 20×20×2.5 m^3. The main objective of these simulations was to perform upscaling to the 1 m scale. Examples of realisations are presented in Figure B-12. The different patters are a result of the different histograms and variograms for the TRCs.

The histogram of the simulated values can be compared to the distribution model used in the simulation, as a step in the validation process. This is performed in Figure B-13 were the match is excellent.

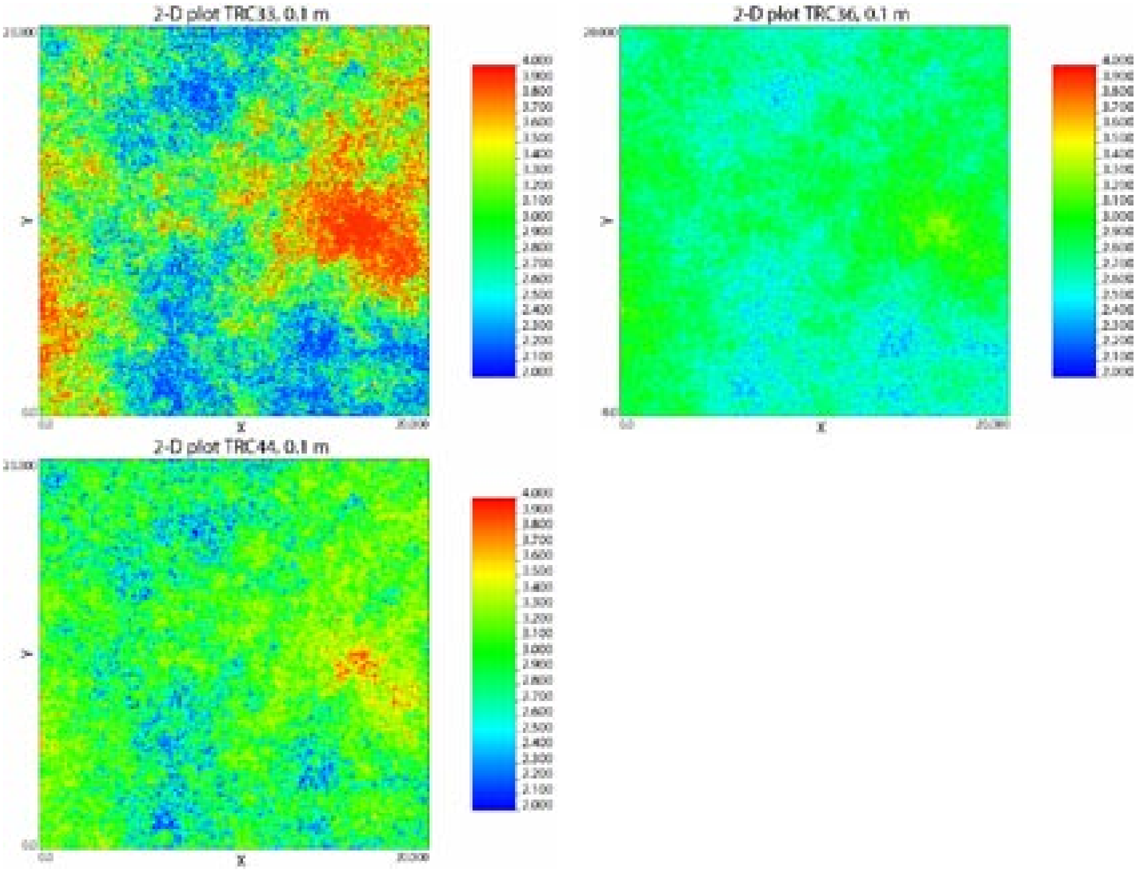

Figure B-12. Examples of realisations from simulations of thermal conductivity for three TRCs (2D slices from 3D realisations). The simulation scale is 0.1 m.

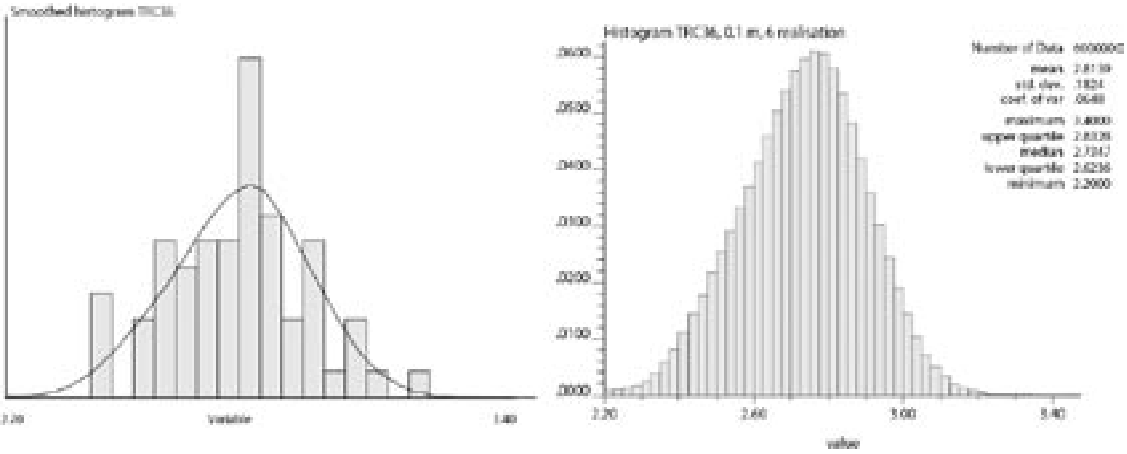

Figure B-13. *Comparison of distribution model (left) and histogram of simulated values (right) for one TRC. A perfect match is expected if the number of simulated values is large (6,000,000 in the example, based on 6 realisations).*

Another step in the validation procedure is to calculate variograms from the simulated values and compared them to the variogram model used in the simulation. This is performed in Figure B-14 where calculated variograms for six realisations are compared to the variogram model. A perfect fit cannot be expected because there is a random component in each realisation.

After upscaling from 0.1 m to 1 m, stochastic 3D-simulations were performed for the 1 m scale. Examples of realisations are presented in Figure B-15. The simulation volume was 100×100×100 m^3, i.e. the same as for the stochastic simulation of TRCs. The main objective was to create realisations that could be combined with the realisations of TRCs.

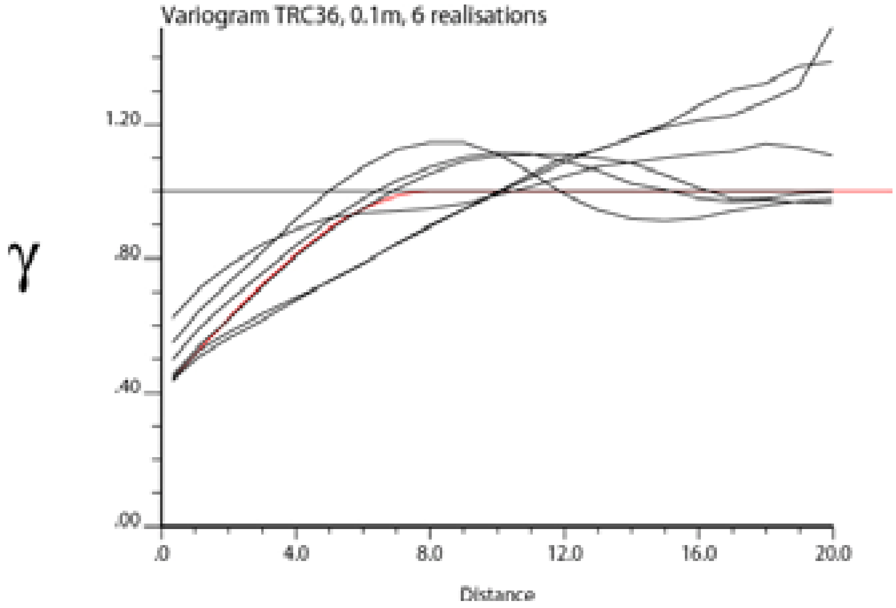

Figure B-14. *Calculated variograms (black) from simulated values compared to the variogram model (red). The simulation scale is 0.1 m.*

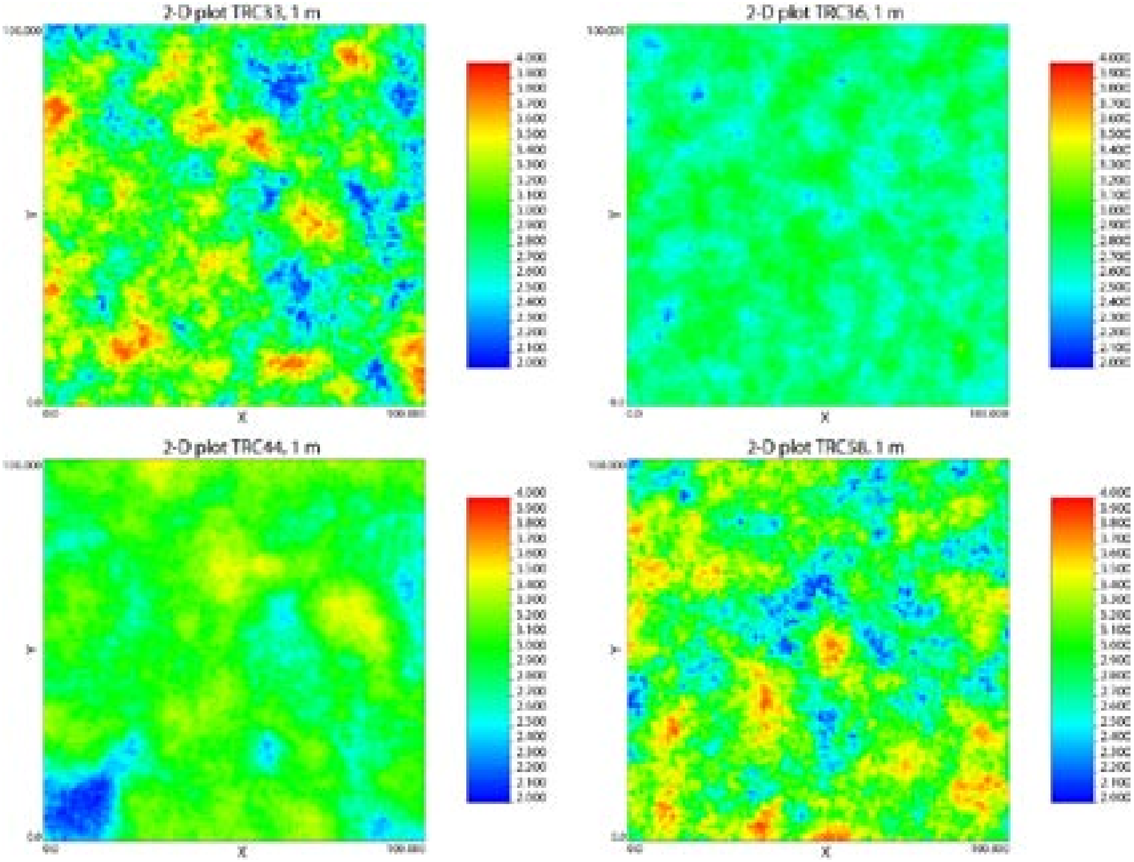

Figure B-15. *Examples of realisations from simulations of thermal conductivity for four TRCs (2D slices from the simulation volume). The simulation scale is 1 m.*

Merging of realisations – step 11

After the simulation of TRCs and the thermal simulations we have one set of realisations of the lithology (Figure B-5) and for each TRC we have one set of thermal realisations (one such thermal realisation is illustrated in Figure B-15 for each TRC). The next step is to merge the realisations of TRCs and the thermal realisations. This is illustrated in Figure B-16. The result is a set of realistic realisations of thermal conductivity that take into account both variability between TRCs and spatial variability within these TRCs; compare Figure B-15 and Figure B-16.

Upscaling of simulation results – step 12

The realisations from the merging have a resolution of 1 m, i.e. the simulation scale. They can be upscaled to the desired scale using the SCA approach. An example of an upscaled realisation from 1 m to 5 m is given in Figure B-17.

The effect of the upscaling is a variance reduction and change in the shape of the histogram. This is illustrated in Figure B-18. Of special importance is the change in the lower tail of the distribution.

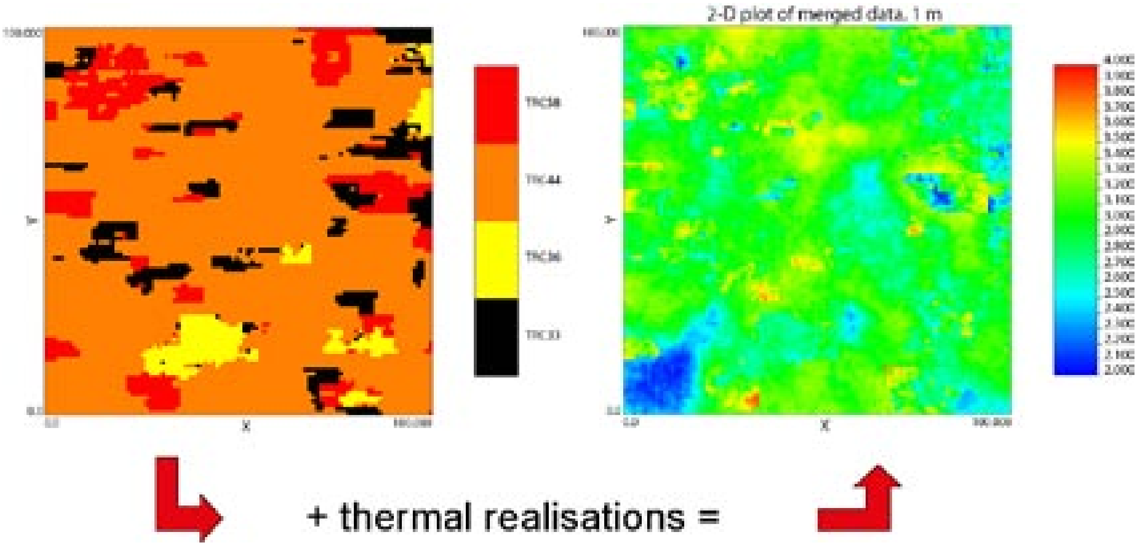

Figure B-16. Merging of lithological realisations (TRCs) and thermal realisations. The realisations are merged using the lithological realisations as masks.

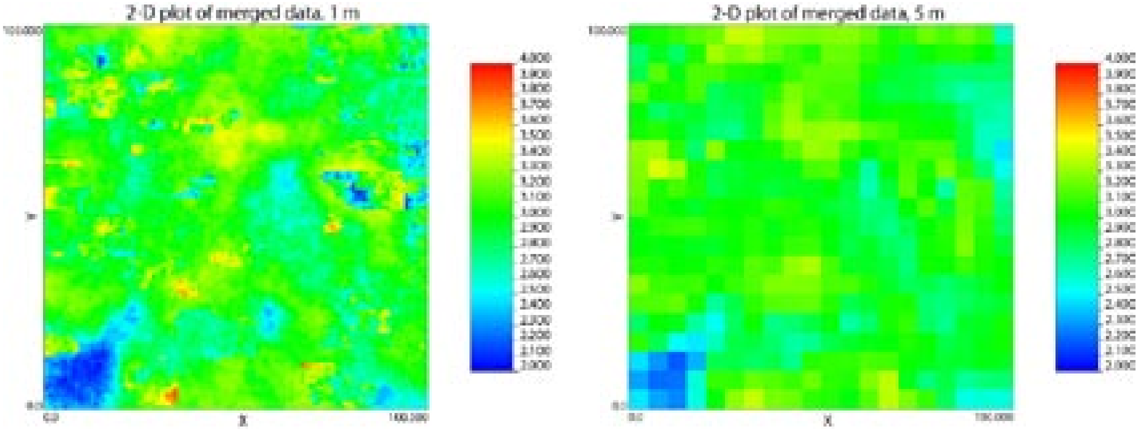

Figure B-17. A 2D realisation of thermal conductivity from simulations with 1 m resolution and the corresponding realisation upscaled to 5 m resolution.

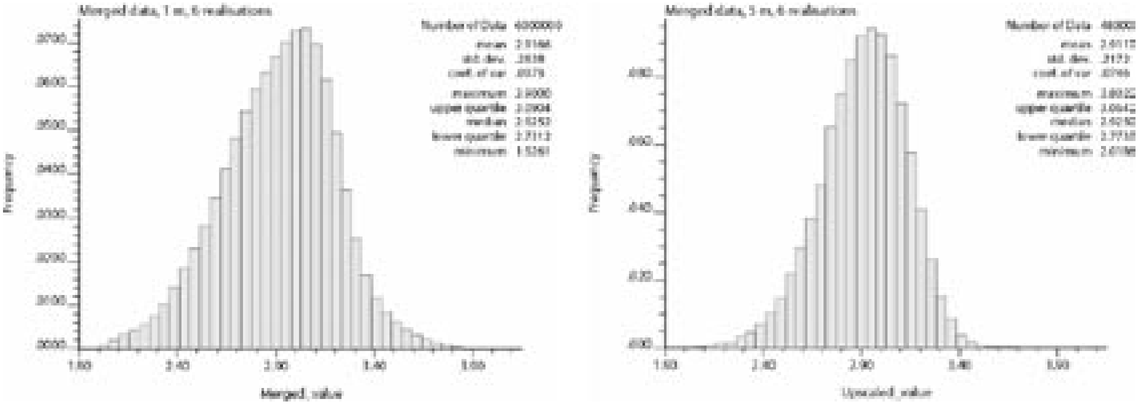

Figure B-18. A histogram of simulated thermal conductivity with 1 m resolution and the corresponding histogram after upscaling to 5 m resolution.

Presentation of results – step 13

The results of the pilot study are the realisations of thermal conductivity exemplified in Figure B-17. These realisations can be described statistically, e.g. with the histograms and statistical parameters in Figure B-18. However, it is possible to proceed with further analysis. Histograms, statistical parameter and confidence intervals can be determined from the simulated values for different scales. In addition, if the number of realisations is large, the probability of encountering values below a threshold can be calculated (if conditional simulation was performed). The realisations can also be used as input to numerical temperature simulations.

Conclusions

The performed pilot study proves that the strategy for thermal modelling presented in Chapter 3 can be successfully applied. The strategy includes powerful geostatistical tools but expert knowledge is also an important part of the methodology. The methodology is transparent and flexible; it can be applied to a wide range of problems in SKB's site descriptive modelling. One important feature is that uncertainties can be managed and also expressed quantitatively. However, the study also illustrates that model uncertainty (for example uncertainty in variogram models) must be considered, although this type of uncertainty can be difficult to quantify.

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