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Methodology for modelling of thermal properties of the Forsmark site

Part 1 – Recommended data and interpretation methods

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Part 1 – Recommended data and interpretation methods

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Preface

A series of methodology reports support the programmes for investigation and modelling during the execution of planned underground constructions at Forsmark. The series includes the following disciplines: geometric modelling of ground elevation and regolith, deterministically modelled geological structures, discrete fracture network (DFN) modelling (stochastic, semi-stochastic and deterministic modelling of structural-hydraulic fracture data), rock mechanics modelling, thermal properties modelling, integrated hydrological and hydrogeological modelling, hydrogeochemical modelling, and transport modelling. Report numbers (ID), acronyms, and titles are shown below. The acronyms are recommended for internal referencing.

ID	Acronym	Title
R-20-10	DGMM	Methodology for deterministic geologic modelling of the Forsmark site.
R-20-11	DFNMM1	Methodology for discrete fracture network modelling of the Forsmark site. Part 1 – Concepts, Data and Interpretation Methods.
R-20-12	DFNMM2	Methodology for discrete fracture network modelling of the Forsmark site. Part 2 – Application examples.
R-20-13	RMMM	Methodology for rock mechanics modelling of the Forsmark site.
R-20-14	HGMM	Methodology for hydrological and hydrogeological modelling of the Forsmark site.
R-20-15	HCMM	Methodology for hydrochemical modelling of the Forsmark site.
R-20-16	ERMM	Methodology for elevation and regolith modelling of the Forsmark site.
R-20-17	TRPMM	Methodology for site descriptive and safety assessment transport modelling of the Forsmark site.
R-20-18	THPMM1	Methodology for modelling of thermal properties of the Forsmark site. Part 1 – Recommended data and interpretation methods.
R-20-19	THPMM2	Methodology for modelling of thermal properties of the Forsmark site. Part 2 – Background and methodology development.

The methodology for thermal modelling at the Forsmark site is presented in two reports, Part 1 and Part 2. This methodology report (Part 1) is an updated version of previous thermal strategy reports (Sundberg 2003b, Back and Sundberg 2007). The previous versions focused on site descriptive modelling at rock domain level. This third version has an updated objective: To describe a methodology to be used in conjunction to the development of deposition areas of the spent fuel repository at the Forsmark site (the construction and operational phases). The methodology is now more focused on prediction at the local scale, using conditional simulation as a tool. A new definition of Thermal Rock Classes (TRC) at the 1 m scale, that better corresponds to the geological classification of rock, has also been included. The principal steps in the methodology (Chapter 5) is slightly revised compared to the previous versions of thermal strategy reports. Background information to the report is compiled in Part 2 (Back et al. 2022).

Valuable background information to the report has been supplied by Lars Rosén and John Wrafter, co-authors of Part 2. A reference group has been connected to the project, with the following persons participating: Diego Mas Ivars, Lillemor Claesson Liljedahl, Peter Hultgren, Anders Winberg, and Eva Hakami. In addition, valuable information has been supplied by Jesper Petersson and Thomas Andolfsson.

Significant contributions to the development of the previous version of the methodology have been made by Johan Andersson, Rolf Christiansson, Lars O Ericsson, Harald Hökmark, Michael Stephens, Assen Simeonov, Raymond Munier, and Peter Dowd.

Summary

The methodology for thermal modelling at the Forsmark site is presented in two reports, Part 1 and Part 2. The objective of this report (Part 1) is to present a methodology for modelling of thermal properties in conjunction to the development of deposition areas of the spent fuel repository at the Forsmark site. The report describes a developed thermal modelling methodology for description, prediction, and visualisation of thermal properties in rock, especially thermal conductivity. This methodology, version 3.0, is an updated version of an earlier strategy applied in the final thermal site descriptive model for Forsmark. Background information on the methodology is presented in Part 2.

Thermal concepts and processes are described, as well as geological aspects of importance for the thermal modelling. In conjunction to this, thermal dimensioning of the repository is discussed. Methods for thermal data collection are presented. Input data to the thermal modelling include models produced in other disciplines, primary data from measurements of thermal properties (see glossary), and primary data from other measurements in the rock mass. Several methods to determine thermal transport properties are described, including field measurements of thermal conductivity in continuous profiles in relevant scale.

The approach for the thermal modelling is to model thermal conductivity (and indirectly heat capacity) in a defined rock volume, using stochastic simulation. The focus is on the most important thermal transport property, the thermal conductivity. The thermal modelling is performed in a ten-step procedure, starting with data collection and data interpretation. Incorporation of expert knowledge is an important part of the approach. The spatial statistical structure of the lithology is modelled, using the concept of Thermal Rock Classes (TRCs). In addition, statistical models of thermal conductivity are developed, followed by stochastic simulations. The result is a large number of equally probable realisations of the spatial distribution of thermal conductivity and heat capacity in the modelled rock volume. These realisations can be used directly as input to the thermal dimensioning.

An important issue of the methodology is that it takes into account the spatial size distribution of rock type bodies and the spatial variability of thermal conductivity within each rock type. Prediction of thermal properties in a specific rock volume can be performed using conditioned data in the stochastic simulations.

In addition to existing data used for earlier Thermal SDMs, simulation volume specific thermal and lithological data are needed, i.e. pilot borehole data. Additional thermal data are preferably field data with the DTS-Heat method at the 1 m scale. If such data is not available, optical scanning is suggested.

Important uncertainties in the thermal modelling are coupled to the availability of data, both the types of data and the amount of data, and the representativeness of data. Bias in data is expected due to non-random location and orientation of boreholes. It is suggested that this bias is reduced by expert elicitation.

Sammanfattning

Metodiken för termisk modellering i Forsmark presenteras i två rapporter, Del 1 och Del 2. Syftet med denna rapport (Del 1) är att presentera en metodik för modellering av termiska egenskaper i samband med byggandet av förvaret för använt bränsle i Forsmark. Rapporten beskriver en utvecklad termisk modelleringsmetodik för beskrivning, prediktion och visualisering av värmeegenskaper i berg, särskilt värmeledningsförmåga. Denna metodbeskrivning, version 3.0, är en uppdaterad version av en tidigare strategi som tillämpades i den slutliga termiska platsbeskrivande modellen. Bakgrundsinformation om metodiken presenteras i Del 2.

Termiska koncept och processer beskrivs, liksom geologiska aspekter av betydelse för den termiska modelleringen. I anslutning till detta diskuteras termisk dimensionering av förvaret. Metoder för datainsamling av termiska egenskaper presenteras. Indata till den termiska modelleringen inkluderar modeller framtagna inom andra discipliner, primärdata från mätningar av termiska egenskaper (se ordlista) samt primärdata från andra mätningar i bergmassan. Flera metoder för att bestämma värmetransportegenskaper beskrivs, inklusive fältmätningar av värmeledningsförmåga i kontinuerliga profiler och i relevant skala.

Angreppssättet för den termiska modelleringen är att modellera värmeledningsförmåga (och indirekt värmekapacitet) i en definierad bergvolym, med hjälp av stokastisk simulering. Fokus ligger på den viktigaste värmetransportegenskapen, värmeledningsförmågan. Den termiska modelleringen utförs i en tio-stegs procedur, som börjar med datainsamling och datatolkning. Inkludering av expertkunskap är en viktig del av angreppssättet. Den rumsliga statistiska strukturen för litologin modelleras med hjälp av konceptet *Thermal Rock Classes* (TRCs). Vidare tas statistiska modeller fram för värmeledningsförmåga, följt av stokastiska simuleringar. Resultatet blir ett stort antal lika sannolika realiseringar av den rumsliga fördelningen av värmeledningsförmåga och värmekapacitet i den modellerade bergvolymen. Dessa realiseringar kan användas direkt som input till den termiska dimensioneringen.

En viktig aspekt i metodiken är att den tar hänsyn till den rumsliga storleksfördelningen av bergartskroppar och den rumsliga variabiliteten av värmeledningsförmåga inom varje bergart. Prediktion av termiska egenskaper i en specifik bergvolym kan utföras med hjälp av konditionerade data i de stokastiska simuleringarna.

Förutom befintliga data, som använts i tidigare termiska platsbeskrivande modeller, kräver metodiken termiska och litologiska data som är specifika för simuleringsvolymen, det vill säga data från pilotborrhål. Ytterligare termiska data är främst fältdata med DTS-Heat-metoden i 1 m-skala. Om sådana data inte är tillgängliga föreslås optisk skanning.

Viktiga osäkerheter i den termiska modelleringen är kopplade till tillgången på data, både typen av data och mängden data, samt representativiteten hos data. Bias i data förväntas på grund av icke-slumpmässig placering och orientering av borrhål. Denna bias föreslås hanteras genom expertbedömningar.

Glossary

The glossary is common to both Part 1 and Part 2.

Boremap is a core and borehole digital mapping system used by SKB during site investigation. All mapped Boremap parameters are stored in SKB database SICADA.

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 at that specific location.

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.

Hard data are data acquired by physical measurement, such as primary data; see *soft data* for comparison.

Heat capacity is the capacity for a material to store thermal energy. In the report, heat capacity is used in a general manner, including both specific and volumetric heat capacity.

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.

Rock occurrence is a part of a drill core, with the same rock, having a length less than 1 m. It is used in Boremap for fine-scale classification of lithology (cf Rock type).

Rock type is defined in a section of drill core with a length larger than 1 m. It is the rock type that has the largest proportion within the interval: Each rock used in Boremap has a SKB Rock type ID number, e.g. 101057 for granite to granodiorite, according to SKB rules for naming of rock types (SKB MD 132.005).

Rock unit is a 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 scale is the size of a grid cell in the simulation, i.e. the resolution of the model.

Simulation volume is the rock volume that is modelled, i.e. all the grid cells in a realisation from a stochastic simulation.

Soft data are data that are acquired in the form of expert knowledge, without physical measurements; see *hard data* for comparison.

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*.

Subordinate rock is a general term and used in different ways depending on scale. Normally the term is used for rock types that are subordinate to the dominating rock type in a rock domain. The term *rock occurrence* is used for specific reference to sections of rock with borehole lengths less than 1 m.

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 lithological modelling includes the statistical modelling of TRC lithology and the stochastic simulation of TRC lithology.

Thermal properties are a broader concept than thermal transport properties and includes both properties and state variables. Thermal transport properties encompass thermal conductivity, thermal diffusivity and heat capacity. Thermal properties also include temperature and the coefficient of thermal expansion, see definitions in Section 2.1. The stochastic modelling in Chapter 5 is restricted to the parameter thermal conductivity but there is a relationship between thermal conductivity and heat capacity, which implies that heat capacity also can be characterised by this approach. The other thermal properties are only described by data.

Thermal Rock Class (TRC) is a concept defined in this report. There are many rock types, but simplifications are required in the modelling and therefore thermal rock classes are defined. Each TRC will have a defined distribution and correlation structure of thermal conductivity values.

Thermal transport properties See explanation in "Thermal properties" above.

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.

TRC lithology is the result of classifying lithological data into Thermal Rock Classes (TRCs). Thus, TRC lithology is equivalent to the lithology expressed as TRCs for the purpose of thermal modelling.

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 sometimes even in the mean). 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.

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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. Forsmark has been selected as the site for the final repository for spent nuclear fuel.

Figure 1-1 shows an illustration of the layout for the final repository at Forsmark, design step D2. The total tunnel length is approximately 72 km.

The deposited nuclear waste canisters will emit heat due to radioactive decay and the thermal conductivity distribution in 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 and tunnels 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. Attribution of thermal properties to the bedrock is referred to as thermal modelling. In this work, the combined use of measurements and simulations are employed.

Thermal transport properties includes thermal conductivity, thermal diffusivity and heat capacity. The broader concept thermal properties also encompass coefficient of thermal expansion and the state variable temperature.

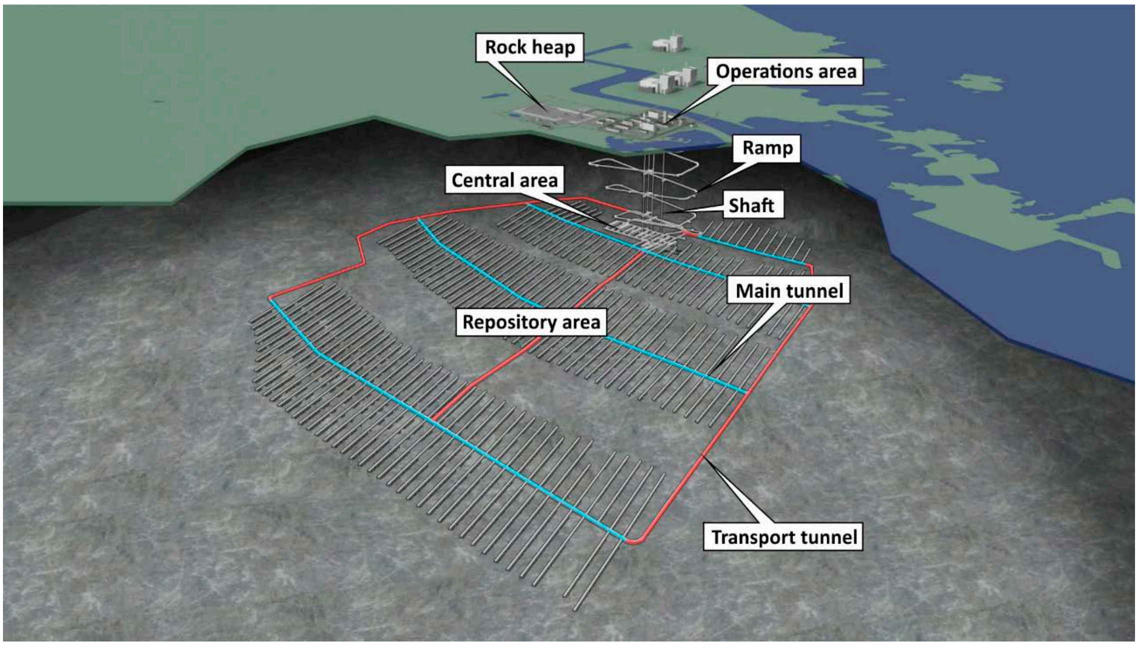

Figure 1-1. *Illustration of the general layout for the final repository at Forsmark, layout step D2. The main parts of the repository are surface facilities, access (ramps and shafts), central area, repository area with deposition areas including main tunnels blue), transport tunnels (red) and deposition tunnels with vertical deposition holes. From Hermanson and Petersson (2022), modified from SKB (2018).*

This report presents a further developed thermal modelling methodology for description, prediction and visualisation. The new methodology, version 3.0, is an updated[1] version of an earlier strategy applied in the final SDM-Site model versions resulting from the surface-based investigations at the Forsmark and Oskarshamn areas (see Back et al. 2007, Sundberg et al. 2008a, b). The previous strategy for thermal modelling is described in detail in Back and Sundberg (2007). The strategy was based on (unconditioned) stochastic modelling of both lithology and thermal properties.

The objective of the previous strategy was mainly to describe the thermal property distribution and other thermal aspects on rock domain level. Focus was on the lower tail of the thermal conductivity distribution. The new developed methodology is adapted so that it can also be applied to local rock volumes on repository depth during the repository construction and operational phases. The repository construction phase involves design and construction of the repository accesses and the central area. More focus is on prediction of the thermal property distribution to enable future optimization of the repository's design. This requires conditioned stochastic simulation and site-specific data.

One important aim of the current development was to improve how the spatial variability in lithology and thermal transport properties[2] is handled. This provides a better basis for characterisation and upscaling of these properties.

1.2 Objectives and scope

1.2.1 General objectives

The objective of this report is to present a methodology for modelling of thermal properties in conjunction to the development of deposition areas of the spent fuel repository at the Forsmark site. General objectives are:

- The methodology is developed for needs connected to the construction and operational phases of a KBS-3 type repository in crystalline rock in Forsmark. The methodology should provide the site-specific properties needed for design and safety assessment.
- The methodology should be adapted to the iterative and integrated character of the preliminary operational programme for detailed site investigations and site-descriptive modelling in conjunction with development of deposition areas in Forsmark. Descriptions should be consistent with those made in other disciplines (mainly geology).
- The methodology is meant to allow full transparency of data gathering, management, interpretations, analysis, and the presentation of results. Spatial variability, as well as conceptual and data uncertainty due to sparse data, errors, and epistemic uncertainty, should be handled and illustrated.

1.2.2 Specific objectives for thermal modelling

The aim of the thermal modelling is to model the thermal properties spatially (3D) for a defined and limited rock mass. 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 4). The stochastic modelling in Chapter 5 is restricted to the parameter thermal conductivity. However, there is a relationship between thermal conductivity and heat capacity, which implies that heat capacity also can be characterised by this approach, as discussed in Section 5.11.

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

[2] The thermal property distribution must be characterised in a proper way without the assumption of a normal distribution. 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.

There are three specific objectives for the thermal stochastic modelling:

- Description: statistical description of thermal conductivity and heat capacity in a defined rock volume.
- Prediction: prediction of thermal conductivity and heat capacity in a defined rock volume (basis for design and adaptation of layout of different underground openings).
- Visualisation: visualisation of the spatial distribution of thermal conductivity and heat capacity.

The focus in this report is on statistical description and prediction, which are the most relevant objectives during the construction and operational phases of the repository. The approach to reach these objectives is described in Section 5.1. The result of applying the methodology presented in Chapter 5 is a set of equally probable realisations of thermal conductivity and heat capacity.

In addition, the methodology 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 must comply with requirements from repository design and safety assessment (safety after closure).

1.2.3 Scope for thermal modelling

Statistical description

Possible results of statistical description are:

- Histograms and statistical parameters of the thermal conductivity and heat capacity distributions for the modelled rock volume, including associated uncertainties.
- A set of equally probable realisations of thermal conductivity and heat capacity.

An important use of the statistical description is to examine and verify that new modelling results are consistent with previous results. The thermal conductivity realisations can be used in the thermal dimensioning of the repository; see Section 2.5.2.

Statistical description can be performed with either conditional or unconditional simulation.

Prediction

Prediction of thermal conductivity is important during the operational phase of the repository. Of special interest is to predict the thermal conductivity between deposition tunnels and around deposition holes. Prediction will be most efficient when conditional stochastic simulation is performed on both lithology and thermal conductivity. This implies that simulated rock types will correspond to the rock types that have been confirmed in boreholes or tunnels, and that simulated thermal conductivity values will correspond to measurements. Possible results are:

- A set of equally probable realisations of thermal conductivity in the modelled rock volume, honouring measurements at specific locations.
- A statistical distribution of possible thermal conductivity values at a specific location in the simulated rock volume. This can also be expressed in terms of confidence intervals.
- A set of equally probable realisations of lithology in the modelled rock volume, honouring rock types at specific locations.

These results can be used to calculate uncertainty in predicted values at specific locations, and thermal conductivity and heat capacity at a larger scale at specific locations, including associated uncertainties. This makes possible the successive adaption and optimisation of the repository design relative to conditions met.

The most obvious use of the thermal modelling results is for medium and long-term thermal behaviour (following backfill and closure) as part of the thermal design and safety analysis of the repository. In Section 2.5.2 there is a description of how the created realisations can be utilized in the thermal dimensioning.

Another important issue is to control that temperature rise is avoided in the repository during construction. Influence on the temperature start conditions for the canisters will influence the design of the repository. To maintain heat balance, controlled temperature measurements is probably an effective action. However, modelling may be useful to understand the causes to a possible unexpected temperature rise.

Visualisation

Visualisation is mainly for communication purposes. It can be performed in 3D for:

- Individual realisations of geology.
- Individual realisations of thermal conductivity and heat capacity.
- Calculated uncertainties, expressed as confidence intervals, prediction errors etc.

3D visualisation of specific rock volumes can enhance analysis of geological and thermal properties, as well as facilitate communication. Visual presentations can be updated as more and more data are collected, thus supporting a successively evolving repository during the construction and operational phases.

2 Thermal concepts and processes

2.1 Definitions

Thermal conductivity and heat capacity are needed to describe the thermal transport process. The thermal 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 even out temperature differences. It is defined as the ratio between thermal conductivity and volumetric heat capacity:

$$\boldsymbol{\kappa} = \boldsymbol{\lambda} / (\boldsymbol{\rho} \cdot \boldsymbol{c}) \quad (2\text{-}1)$$

The geothermal gradient [ºC/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 parts of the Earth. The natural geothermal heat flow in Sweden is mainly a vertically oriented process and is governed by the equation:

$$\boldsymbol{q} = \boldsymbol{\lambda} \cdot \left(\frac{\boldsymbol{dT}}{\boldsymbol{dz}}\right) + \int \boldsymbol{A}(\boldsymbol{z})\boldsymbol{dz} \quad (2\text{-}2)$$

where dT/dz is the geothermal gradient and A the internal heat production. The temperature change as a function of depth below the ground surface.

The internal heat production A [mW/m^3] is defined as the heat produced within the rock mass due to nuclear decay.

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

2.2 Thermal properties of rock

The thermal site descriptive model should include description of the temperature distribution, boundary conditions and other thermal properties of the rock mass. The temperature is the result of the thermal processes being active 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 treated are listed in Table 2-1.

The thermal properties are measured for the intact rock, often as small-scale measurements. Discontinuities in the form of fractures influence the thermal properties. However, this influence is assumed to be small within the repository area, due to low porosity and low hydraulic conductivity of the rock mass, and is therefore neglected. Only heat conduction and heat capacity are included in the thermal modelling.

Table 2-1. Listing of thermal properties and parameters that will be described by or involved in the thermal modelling strategy. For definitions, see Section 2.1.

Parameter	Unit
Thermal transport properties	
Thermal conductivity	W/(m·K)
Heat capacity	J/(m^3·K) or J/(kg·K)
Thermal diffusivity	m^2/s
Temperature	
Temperature in the rock mass	ºC
Temperature gradient	ºC/m
Boundary conditions	
Geothermal heat flow	W/m^2
Temperature and climate conditions at the ground surface	ºC
Other thermal properties	
Internal heat production in the rock	μW/m^3
Thermal expansion of rock	m/(m·K)
Other relevant properties	
Density and porosity	kg/m^3 and %

2.3 Natural thermal processes

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

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

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

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 (^{40}K) in the rock itself.

In the rock mass, the thermal transport mainly results from conduction (local convection due to groundwater flow in fractures or fracture zones may exist but with extremely low conductivities and small gradients in the repository after closure this is negligible). In the thermal modelling the heat transport is thus assumed to be trough conduction only. Heat transport through radiation can be neglected.

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

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

where

T = temperature,

t = time, and

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.

2.4 Scales of thermal processes in the repository

2.4.1 General

All modelling will consider a certain scale, and for SKB purposes a nomenclature for different applicable scales has been developed to enable consistent terminology. These scales are illustrated in Figure 2-1. Depending on the discipline, some scales are more relevant than others.

Thermal modelling during SDM were performed with data in the facility scale and the realisation output approximately in the tunnel scale but with resolution in the 1 m scale. However, thermal data may represent much smaller scales. Therefore, the thermal modelling may involve upscaling to the simulation scale (the resolution of the thermal model).

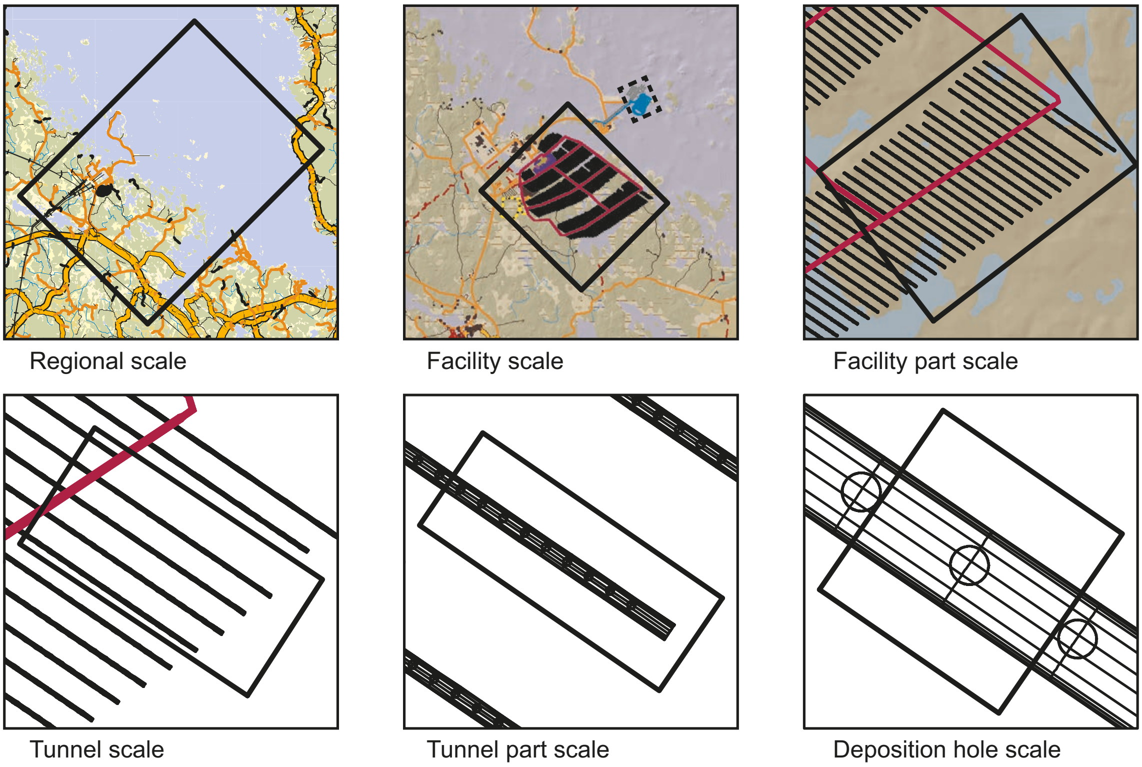

Figure 2-1. *Illustration of model scales applicable to construction and operation of radioactive waste disposal facilities in the Forsmark area including development of site descriptive models (SDM).*

2.4.2 Scales influencing the canister temperature

The "global" temperature field around a repository (local scale) 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 spatial thermal property distribution are lower compared to the deposition hole scale.

The temperature field in the deposition hole scale and the tunnel scale 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).

The sensitivity in canister temperature to changes in the thermal properties is highest for the area closest to the canister. However, also thermal properties at a distance may influence the 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.

In order to analyse the scale (see *Simulation scale* in the glossary) at which variations of thermal conductivity becomes significant for the temperature on the canister, a numerical study based on rock thermal conductivity distribution have been made (Sundberg et al. 2005b). 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 2-2) and for larger scales increased even further. Consequently, the maximum temperature and the temperature development are influenced by thermal conductivities for a range of scales.

During the thermal site descriptive modelling, the question of what scale the thermal modelling result would be presented in became central along with how the result would be used as input to the design of the repository. After analysis of the problem, it was found that all scales affected the canister temperature even if sensitivity of the thermal properties close to the canister were highest.

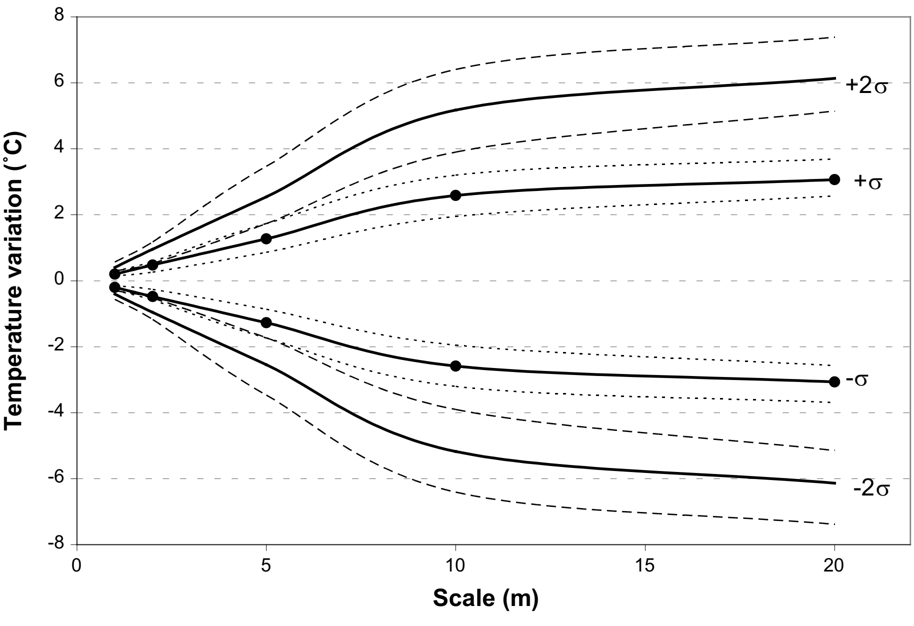

Figure 2-2. *Simulated canister temperature variations at one and two standard deviations based on average values for each scale. Thermal conductivity values are randomly assigned from a normal distribution for each scale (mean: 2.8 W/(m·K), std: 0.35 W/(m·K). The dotted lines show the temperature variation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

Important conclusions:

- Using mean of thermal properties for thermal dimensional properties is only relevant if the rock is homogeneous and all spatial variations are evened out in a smaller scale than the scale relevant for the heat dissipation from the canister. Since the rock types in Forsmark are inhomogeneous at these scales the use of mean thermal properties are not relevant.
- The scale relevant for the temperature increase of the canister is time dependent. In the beginning of the heating process only a small volume around the canister influences the temperature increase. With a gradually longer heating time, a larger and larger rock volume affects the temperature development of the canister. Consequently, the maximum temperature and the temperature development are influenced by thermal conductivities for a range of scales.
- As a consequence, the strategy for thermal dimensioning of the final repository (Hökmark et al. 2009) involved the direct use of a large number of thermal realisations, created in the thermal modelling, in a numerical model simulating a repository.

2.5 Thermal dimensioning of the repository

In the Swedish KBS-3 concept for geological disposal of spent nuclear fuel, canisters are deposited in vertical deposition holes in the floor of horizontal tunnels, see Figure 1-1. The canisters are surrounded by bentonite clay for isolation and mechanical protection. The canisters containing spent nuclear fuel generate heat due to radioactive decay. The heat will increase the temperature in the repository. The peak temperature of the bentonite buffer must not exceed 100ºC for any of the deposition holes. This temperature limit is one important factor when deciding the repository layout, i.e. the distance between deposition holes and deposition tunnels.

The natural temperature field will already be disturbed during the construction of the repository, related to ventilation, machines and lighting etc. Temperature increase influences the start conditions for the deposited canisters, and therefore the thermal dimensioning, and should be avoided.

2.5.1 The strategy for thermal dimensioning step D2

The strategy of the thermal dimensioning of the repository is described in Hökmark et al. (2009) and forms a basis for the guidelines for underground design step D2 of the repository (SKB 2009).

The strategy for thermal dimensioning describes how thermal properties were used in the design process of repository layout and provides a better understanding of how the developed thermal methodology can be used during the repository's operational phase. A brief summary follows.

The strategy is focused on design step D2 for which a set of design premises has been specified, e.g. the spacing between tunnels is fixed at 40 m. In addition, there should not be any optimization of the layout, i.e. the canister spacing should be set to the same value everywhere in each rock domain such that the temperature criterion is met for every canister.

The hottest canisters will be those deposited in dry deposition holes in low-conductivity rock in central parts of the deposition areas.

In the flowchart in Figure 2-3 the dimensioning procedure is summarized and involves different steps. A first trial value of canister spacing (5) is established from an analytical approach (4) with the thermal model (1) as input. There are uncertainties in input data as well as systematic over- and underestimates. Therefore, a margin (3) to the 100 °C criteria is established.

The thermal model (1) is the basis for the thermal dimensioning. The large number of 3D realisations that are the output from the thermal modelling (6) can be used directly as input to the numerical approach (7).

The 3D numerical method takes spatial variations and autocorrelations in the thermal properties into account by establish an example repository with deposition tunnel and 9 heated canisters in the 3D realisations. In this way all scales of thermal conductivity are taken into account when the maximum bentonite temperature is calculated.

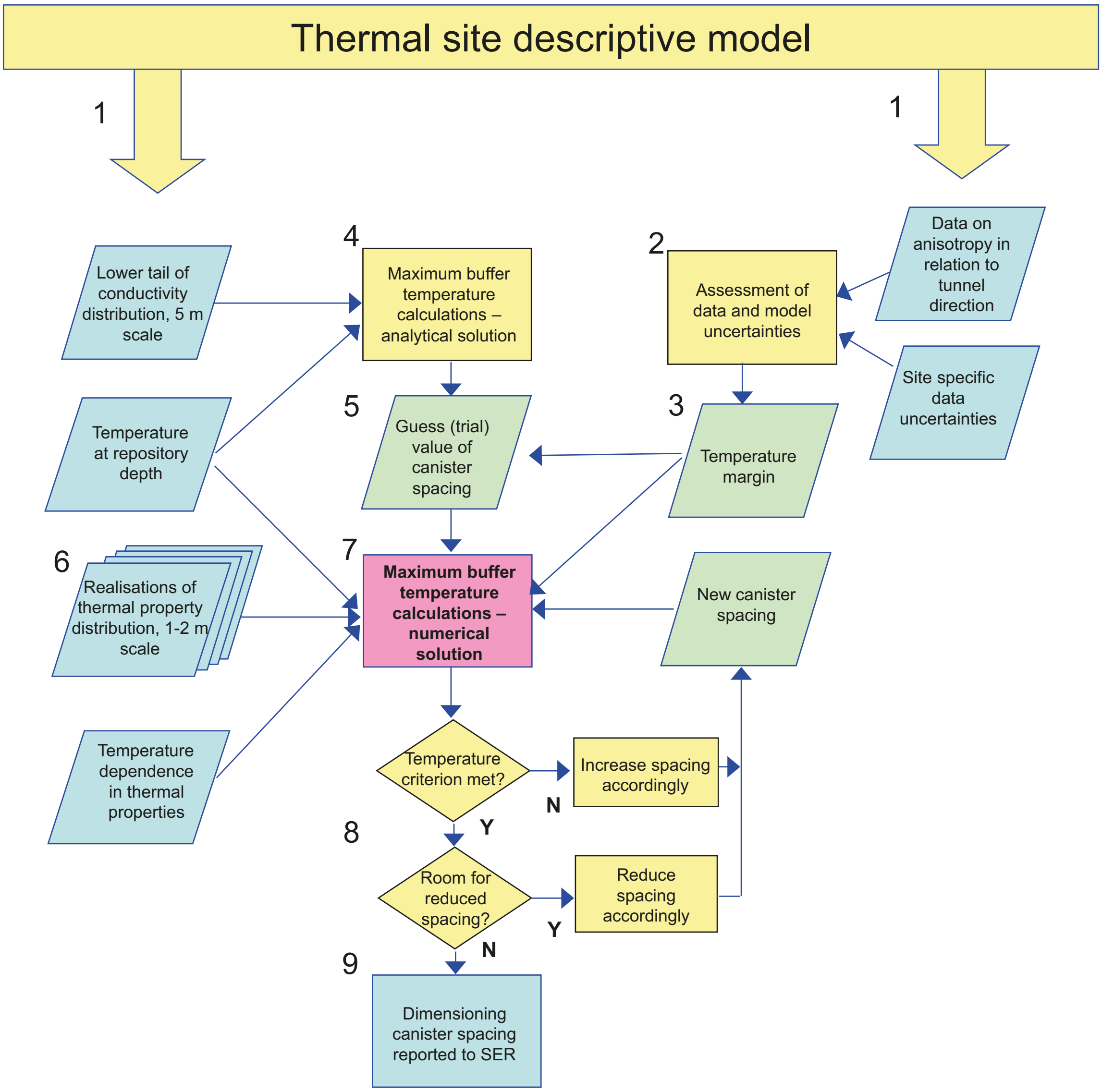

Figure 2-3. *Schematic description of the strategy for thermal dimensioning of the repository (from Hökmark et al. 2009). Possible optimization measures are not included in the scheme. The last step 9 contains a reference to SER, which is an abbreviation of the Site engineering report Forsmark and contains guidelines for design step D2 (SKB 2009). Note the difference in scope and outline compared to Figure 5-1.*

2.5.2 Thermal dimensioning of the Forsmark layout D2

The thermal dimensioning of the Forsmark layout is presented in the site engineering report for Forsmark (SKB 2009). The dimensioning of the canister spacing were performed with input from realisations of the thermal conductivity distribution in domain RFM029 and domain RFM045 (Back et al. 2007, Sundberg et al. 2008b).

The thermal dimensioning follows the flowchart in Figure 2-3. Insight into the thermal dimensioning result increases the understanding of how the results from the thermal model may be used during the operational phase. It also contains interesting results about dimensioning rock type distribution. The following description focuses on steps 7–9 in the flowchart; maximum buffer temperature calculations with the numerical solution and realisation input.

Overview of the numerical approach

About 500–1 000 realisations were created for each rock domain in Forsmark during the site investigations. Each realisation contains typically 125 000 cells at 1 m^3 (50 × 50 × 50 m rock volumes). Each cell contains information of thermal conductivity and heat capacity. A code identifying the actual Thermal Rock Class (TRC; see Section 5.4.3) is also connected to each cell. The realisations are used as input to a numerical calculation model with one deposition tunnel and 9 canisters. The realisations are in a local coordinate system in order to take the geological anisotropy into account. In the numerical model, data is collected from each cell in a realisation and transformed into the coordinate system for the numerical model.

In a pre-processing step, the realisations are ranked in an expected order, from the realisation with the lowest thermal conductivity (based on four successively increasing volumes around each canister) to the realisation with the highest thermal conductivity. The numerical calculations are made on the first ranked realisations.

One of the main benefits with the numerical approach is that it includes all scales of the thermal rock property distributions. Therefore, there is no need to try to find the right percentile of the rock domain conductivity distribution in a "relevant" scale that is dimensioning for the domain.

The ranking procedure

As the numerical simulations are time-consuming, it would be helpful if a certain number of potential worst cases could be found by a screening of the different rock thermal conductivity realisations in the repository. In order to achieve this objective, the geometric mean of the rock thermal conductivity was calculated in four zones around each canister.

The first zone extends from the rock wall to a distance of 2.5 m from the canister. The zones are calculated as a cylinder. The volumes of the four zones are approximately 170, 800, 5 030 and 12 230 m^3. Based on the calculated heat flow, the weighting coefficients are approximately 0.4, 0.25, 0.25, and 0.1 for the four zones respectively (Hökmark et al. 2009).

The resulting weighted thermal conductivities around each of the five central canisters in each realisation were used as ranking parameter. The first ranked realisation has the lowest weighted thermal conductivity and should consequently also have the highest calculated temperature if the ranking procedure picked the realisations in the right order. However, a perfect match between ranking based on weighted thermal conductivity and temperature cannot be expected. Selecting the first ten ranked realisations was judged to be a reasonable precaution to ensure that the realisation with the lowest thermal conductivity had been included in the numerical temperature calculations during the thermal dimensioning of the Forsmark layout (SKB 2009).

In the ranking procedure, also the percentage of each rock type were calculated for the four zones, for each canister in each realisation. This means that the ranking procedure gave data on the rock types and mean conductivities that affected the temperature on each of the 9 000 simulated canisters in rock domain RFM029 (9 canisters × 1 000 realisations) and 4 500 canisters in rock domain RFM045 (9 × 500).

Results

The thermal dimensioning resulted in canister spacing 6 m and 6.8 m in domain RFM029 and RFM045, respectively (SKB 2009). The calculated bentonite temperature at the hottest canister in domain RFM029 was only 0.3 °C below the temperature criteria. It can also be concluded that increased ranking in general corresponds to lower maximum bentonite temperature. However, it is possible to develop the ranking procedure further.

The amount of amphibolite in the zone closest to the canister (170 m^3) for the first ranked realisations, and the mean weighted thermal conductivity in these volumes, were reported in SKB (2009).

In domain RFM029 the amount of amphibolite in the zone varied from 67 % to 1 % for the hottest canister in each of the ten first ranked realisations. In domain RFM045, the corresponding numbers were from 100 % amphibolite to 76 %. Especially in domain RFM029 rocks other than amphibolite are dimensioning for the temperature, probably low conductive varieties of rock type 101051, Granite, granodiorite and tonalite.

2.5.3 Possible optimization during the operational phase

The design criteria for layout D2 meant that the hottest canister was dimensioning for all canisters. The majority of the canister positions will be deposited in volumes of rock that dissipates heat much better than the low-conductivity rock that controls the layout decisions. There are also many hundreds of positions near the tunnel ends that would get buffer temperatures lower than the threshold regardless of the local heat transport conditions. This means that there is significant room for layout optimizations (Hökmark et al. 2009).

The potential for optimization were illustrated by Lönnqvist (2018). In this study a numerical model is used where the rock mass is simplified to consist of two materials; low-conductive dykes of amphibolite in a mean conductive rock mass. The vertical dykes were parallel to the deposition tunnel and situated on each side of the tunnel. Lönnqvist showed that the canister temperature in the rather extreme geological model modelled did not exceed the temperature criteria and thus confirmed the thermal dimensioning.

The ranking procedure during the thermal dimensioning (SKB 2009) gave rise to a large amount of dimensioning data. Processing such information should provide an improved understanding of the possibilities for optimization in the repository. The dimensioning concept from Figure 2-3 may be used during the operational phase and the ranking procedure may be developed.

3 Thermal geology

3.1 General

The methodology for deterministic geological modelling is described in DGMM (Hermanson and Petersson 2022). The methodology utilizes the foundations laid out in Munier et al. (2003) and was developed during the site descriptive modelling in Laxemar and Forsmark (e.g. Stephens et al. 2007). The developed methodology is focusing on the development of the repository and handles the type of information that will be available during the construction and operational phase of the repository, namely borehole and tunnel data.

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.

In the updated geological methodology, object-based modelling is being introduced, capable of handling large amounts of data. The main information components are the geoscientific single-hole interpretation and the geological single-tunnel interpretation, the latter being a new method which will form an additional structured building block to the subsequent 3D modelling process.

Of special interest for the thermal model is the lithological description, Boremap data, the geometric interpretation in the geological site descriptive model, and expert knowledge.

The rock mass contains discontinuities in a wide size range, from micro-fractures in single minerals to regional deformation zones. From a thermal point of view, the micro-fractures are included in the intact rock and are determined as porosity in 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.

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 have similar properties. 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. Rock domain is a region of the rock mass for which the properties can be considered essentially the same in a statistical sense. In the geological model, several rock units are assembled into rock domains; see Hermanson and Petersson (2022).

The developed geological modelling (Hermanson and Petersson 2022) opens up for a sub-division of large-scale rock domains in the repository as a basis for thermal modelling.

In Figure 3-1 the geological modelling concept is presented for repository areas. Expert knowledge from the geological modelling constitutes important input to the thermal modelling, especially with respect to geometric conditions.

In the thermal modelling, properties are modelled for the different rock domains or limited parts of rock domains. For practical reasons, mainly for simplifying the stochastic simulations, different rock types with similar thermal properties are put together into Thermal Rock Classes (TRCs); see Section 5.4.3. This definition of Thermal Rock Classes is more in accordance with the geologists' classification of rock than previously definitions; see Back et al. (2022).

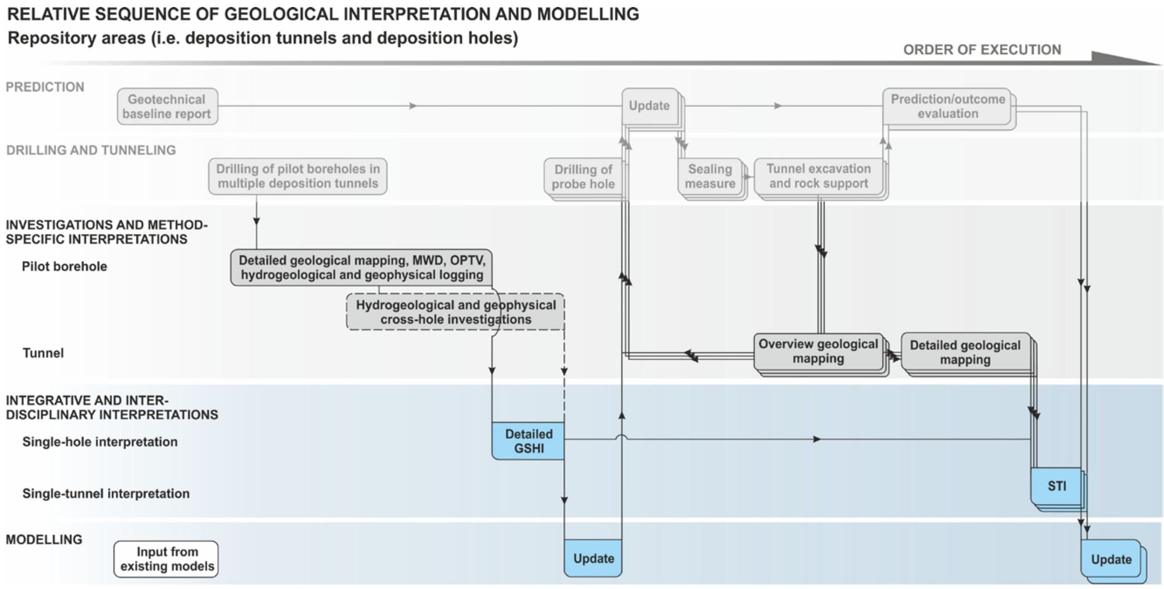

Figure 3-1. *Overview of the geological interpretation and modelling for repository areas (Hermanson and Petersson 2022).*

3.2 Specific rock types and geometrical aspects

The new developed methodology for thermal modelling is adapted so that it can also be applied to limited rock volumes during the operational phase. More focus is on prediction of the whole thermal property distribution to enable future optimization of the repository design. However, low conductive rock is still an important issue.

The dominant rock in RFM029 is a metamorphosed, medium-grained granite to granodiorite (101057, c 74 % of the domain volume). Corresponding dominant rock types in domain RFM045 are aplitic metagranite (101058) and medium-grained metagranite (101057). They constitute 49 % and 18 % of the domain respectively (Stephens et al. 2007). Figure 3-2 shows an overview of the rock domain distribution in the repository area.

The main low thermal conductive rocks are amphibolite and granodiorite to tonalite. The amphibolites appear both as elongated bodies with limited thickness and as larger bodies, lumps. The amphibolites are often orientated parallel to the main horizontal stress and to the foliation and lineation. The amphibolites bodies are larger in domain RFM045 compared to RFM029 (Stephens et al. 2007).

Rock type granodiorite to tonalite appears to be more difficult to predict than amphibolite. It appears as fewer and larger bodies or passages, from a few metres up to tens of metres (Petersson J 2020, personal communication).

A third subordinate rock is pegmatite. This is however not a low-conductive rock. Pegmatites are of different ages. Older pegmatites often appear as veins in parallel with the foliation (concordant), mainly in the dominating rock type granite to granodiorite which can be experienced as striped. Younger pegmatites can be both concordant and discordant to the foliation and appear to a greater extent as dykes (Stephens et al. 2007, Petersson J 2020, personal communication).

During the construction of ramp and central area valuable information will be gained, especially of the geometrical distribution of e.g. amphibolite and granite to tonalite (101051). For the latter, better understanding is possible regarding to what degree bodies are homogeneous with respect to mineralogical composition (tonalitic, granodioritic, or granitic) or the bodies are a mixture of these. Also, a better understanding of the size distribution of rock bodies of granite to tonalite is possible.

The deposition tunnels will be aligned parallel to subparallel to the foliation and maximum horizontal stress. Since several important rocks have their major extent parallel to foliation, the information from most tunnels and boreholes are expected to be biased for these. This poses a challenge and requires close collaboration with geology in order to obtain expert knowledge for the thermal lithological modelling.

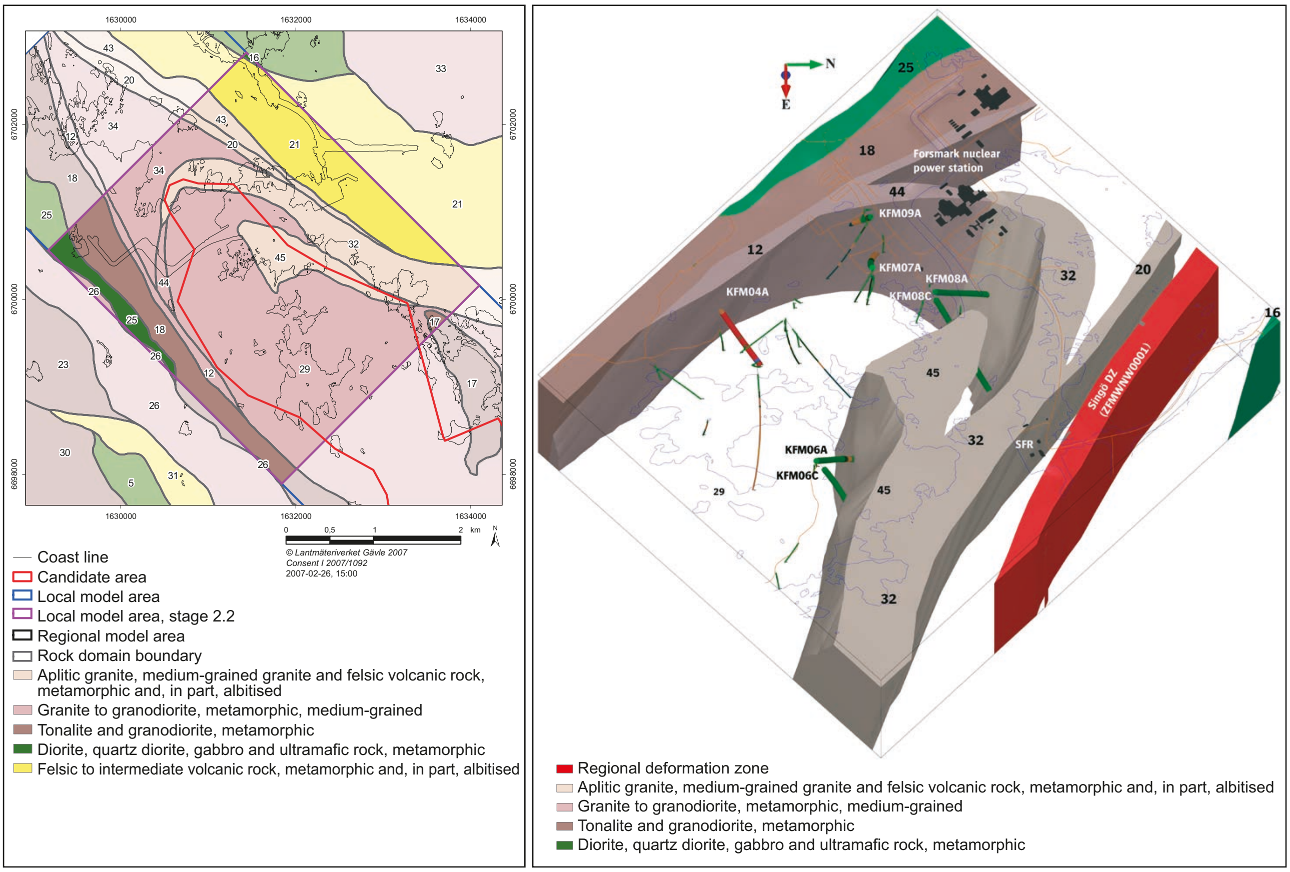

Figure 3-2. *Overview of the rock domains in Forsmark with RFM029 (marked 29) and RFM045 (marked 45) in a map of ground surface and in a 3D model where RFM29 is hidden (empty). The investigation boreholes are also included in the model. From Stephens et al. (2007).*

3.3 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 a fracture zone oriented perpendicular to the heat flow can be considered non water bearing, it can act as a barrier to the heat flow.

Thermal properties of fracture zones can be evaluated from geological and hydrogeological description, and from geophysical data. However, fracture zones are assumed not to be accepted close to the deposited canisters (of reasons related to groundwater transport criteria). The thermal influence from fracture zones foreseen on the local temperature field at the canisters will therefore be small. Consequently, fracture zones are not included in the thermal stochastic modelling approach; see Section 5.1.

3.4 Interdisciplinary interpretation

Close cooperation between geology and thermal modelling teams is necessary in order to make the best use of available knowledge. The need for cooperation depends largely on available data.

In addition to general cooperation, interaction is at least required regarding:

- Expert knowledge to minimize the significance of bias in the thermal lithological modelling. Such bias can be expected due to the orientation of boreholes, subparallel to foliation; see Section 3.2 (connected to Sections 5.4.4 and 5.4.5, preparing and classifying lithological data).
- Potential sub TRCs based on result of geological single hole interpretation. For example: alteration that influence the thermal properties may suggest subdivision of TRCs to improve the thermal modelling (connected to Section 5.4.3).
- Identifying and preparing data for potential thermal sub domains, based one identified sub domains in the geological modelling.
- Feedback to the geology team based on results from the lithological modelling in the thermal model.

4 Methods for thermal data collection

4.1 Identification of input data and interaction with other disciplines

Identification of input data is an essential part of the thermal modelling strategy. 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. In the earlier strategy, this is described in more detail (Back and Sundberg 2007).

4.2 Relevant scales

The thermal properties vary depending on the scale of observation. Observation scales may range from millimetres or less, up to several meters or more. Heterogeneities and anisotropies 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 represent 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 (Sundberg 1988) is theoretically the appropriate method of upscaling in 3D; see and Back and Sundberg (2007). However, the difference in result compared to the geometric mean is often small for thermal conductivity in rock.

The statistical parameters of the distribution of thermal conductivity values are affected by the upscaling. The mean of the distribution is generally affected only to a small extent. However, the variance and standard deviation are 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. The upscaling process itself involves uncertainties and using data that represents the scale of interest is therefore preferable.

However, the temperature evolution for canisters is influenced by a range of different scales. It is therefore difficult to choose *one* scale that is representative for the temperature development and can be used for detailed adaption of repository design.

4.2.1 Determination of thermal properties in laboratory scale

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 will to a large degree be averaged out at the centimetre scale. Determinations of thermal properties in the laboratory are often made at this scale. However, even for a homogeneous magmatic rock there is always a variation in properties due to chemical variations in the original magma of the orogenesis. 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 large variability will exist at the small scale but not necessarily at a larger scale.

4.2.2 Large scale thermal properties

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).
- DTS (Distributed temperature sensing) using integrated heating (0.1 m – full borehole length).
- Thermal response test (5–100 m).

It is desirable that the field measurement scale is in accordance with the simulation scale (cell size, approximately metre-scale) to avoid upscaling; see Section 4.4.3, Chapter 5 and Back et al. (2022).

4.3 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.

4.3.1 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 4.4.4.

The thermal conductivity of some minerals, for example plagioclase, depends on the chemical composition of the mineral, e.g. the relationship between Ca and Na in plagioclase. The chemical composition is not determined and is therefore an uncertainty factor.

4.3.2 Temperature

Studies of the temperature dependence of the thermal conductivity of common rocks presented in literature have shown a decrease in thermal conductivity with increasing 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.

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 (101057) (Sundberg et al. 2005a).

Heat capacity exhibits large temperature dependence. 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 dimensioning. The temperature also has an influence on the density, in the case volumetric heat capacity needs to be transformed to specific heat capacity.

4.3.3 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-fractures. These micro-fractures 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), see Figure 4-1.

However, thermal conductivity under dry or unsaturated conditions may have up to approximately 10 % lower thermal conductivity compared to saturated conditions, or high pressure (100 MPa) (Walsh and Decker 1966). The maximum rock stress at the deposition hole walls varies with the orientation around the periphery. At the beginning of the deposition it is about 10–120 MPa and increases with the thermal load from canisters (Hakami E 2021, personal communication). All thermal conductivity measurements in laboratory are made on water saturated samples according to the methodology description for determining thermal properties (SKB MD 190.001e ver 3.0), see also Section 4.4.2.

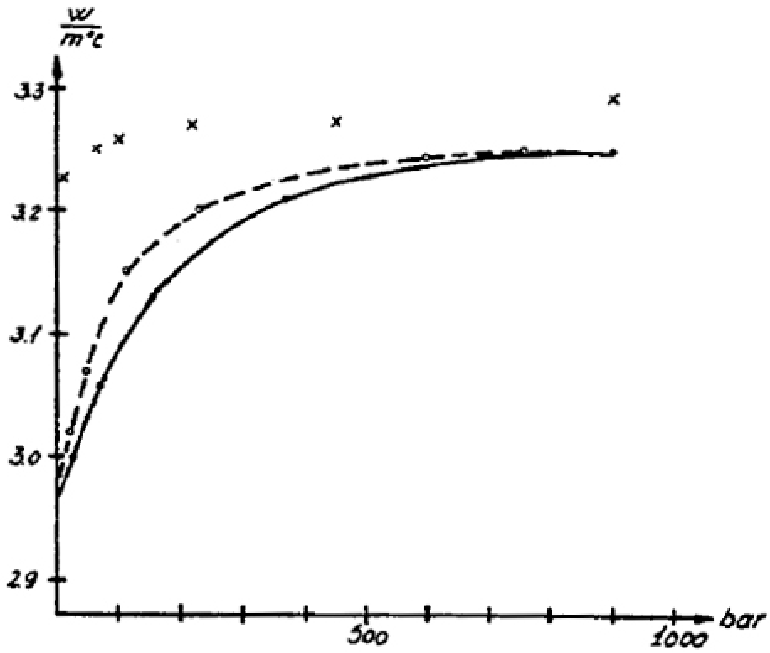

Figure 4-1. *Measured thermal conductivity for a granite sample under axial pressure (rock stress). Data for water-saturated sample are indicated by a cross, while the pressure dependence of a dry sample is shown by dots and circles depending on the rising or falling pressure (Walsh and Decker 1966). 1 000 bar is equivalent to 100 MPa.*

4.3.4 Anisotropy

In anisotropic rocks, the thermal conductivity is different in different directions; see Figure 4-2. This must 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:

$$\lambda = \lambda_x \cdot \cos^2 \varphi + \lambda_y \cdot \sin^2 \varphi \quad (4\text{-}1)$$

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 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 (see also Back et al. 2022):

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, depending on the mineral composition of the rock. 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 mineral orientation of the commonly occurring minerals in a rock, such as quartz and biotite.

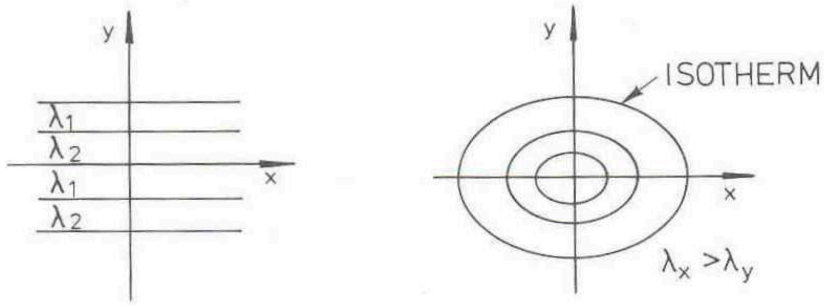

Figure 4-2. *Anisotropy (Sundberg 1988). Thermal conductivity is denoted by λ.*

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 significantly 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 rock bodies, primarily subordinate rocks. These rocks may have preferential directions in space, resulting in anisotropy of the thermal properties. Amphibolites parallel to the foliation and lineation 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.

How anisotropy is handled during the thermal modelling is described in Section 5.13.

4.3.5 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 4-3.

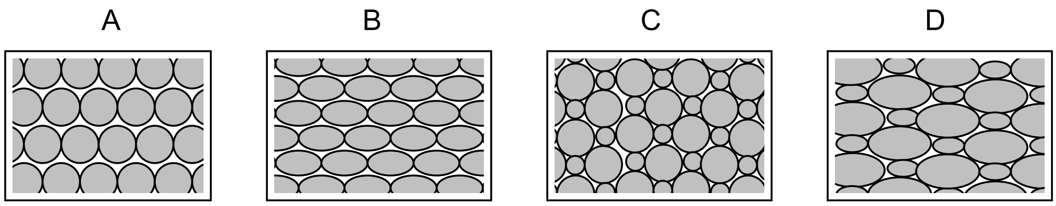

Figure 4-3. *The concepts of heterogeneity and anisotropy: A) homogeneous isotropic material, B) homogeneous anisotropic material, C) heterogeneous isotropic material, and D) heterogeneous anisotropic material (Norrman 2004).*

4.4 Determination of thermal transport properties

4.4.1 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.

4.4.2 Laboratory measurements

TPS method

There are different types of laboratory methods to determine thermal properties; see for example (Sundberg 1988). The recommended laboratory method for the surface-based site investigations was the TPS (transient plane source) method (SKB 2001). It is a transient method, unlike the commonly used divided bar method. The method uses a sensor element with an engraved pattern of a thin metal double spiral. The spiral is embedded in an insulation material and installed between two rock samples. The sensor both emits heat and measures the temperature. It is possible to evaluate both thermal conductivity and diffusivity, and from these entities the volumetric heat capacity is calculated. Depending on desired measurement scale, different sensor sizes can be used. The TPS method is described in more detail by Gustafsson (1991) and in SKB Method description for determining thermal properties (SKB MD 190.001e ver 3.0). 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 thermal penetration depth into the sample depends on the size of the measurement sensor; with standard sensors approximately 10 mm to 14 mm (Sundberg et al. 2005b). TPS measurement are made on water saturated samples according to the methodology description.

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; the latter used for the Finnish site investigations. The comparison was made for 17 samples and showed satisfactory agreement regarding the mean values for all samples but rather large discrepancies for individual samples (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 in relation 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.

Optical scanning

Optical scanning is a transient laboratory method that has the ability to determine the thermal properties of continuous profiles along drill cores and requires no physical contact with the sample. The method was introduced in practical use by Popov et al. (1985). The method contains a heat radiation source (e.g. laser) and infrared temperature sensors that moves with constant velocity along the drill core on a slid, see Figure 4-4.

The penetrating depths can be controlled by the scanning speed and can reach 2–3 cm for high conductive rock types. On the sample surface a thin coating is applied two minimize different optical reflections (Popov et al. 1999a).

By using reference standards with known thermal conductivity, λ_r, aligned with the sample in the scanning direction, the sample thermal conductivity, λ_s, can be calculated simply from λ_r and the ratio of the temperature rise in T_r and T_2:

$$\lambda_s = \lambda_r \cdot (T_r / T_2)$$

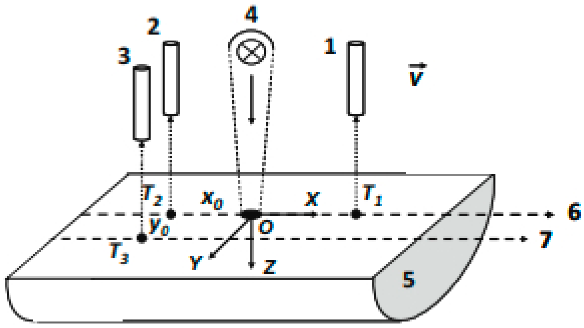

Figure 4-4. *The principle of optical scanning (Popov et al. 2016). V: Velocity; O: area of the heat spot; 1-3: infrared temperature sensors;* T_1*: initial temperature,* T_2*: temperature for thermal conductivity determination,* T_3*: temperature for thermal diffusivity determination.*

It is also possible to calculate the thermal diffusivity with the method by using another temperature sensor at known distance perpendicular to the scanning line/direction; see Figure 4-4. A third temperature sensor is used before the heat source to measure the initial temperature.

The method has been compared with two another well investigated methods, the divided-bar method and the line source method, on many anisotropic samples from gneiss, amphibolite, and other rock types. In general, the deviation in results was within 4 % between the methods and within 2 % for the less anisotropic samples (Popov et al. 1999a).

The method is widely used for example on cores from the Kola super-deep hole project (Popov et al. 1999b) but also in Sweden (Andolfsson 2013). It is one of ISRM's (International Society for Rock Mechanics and Rock Engineering) suggested methods to determine rock thermal properties in laboratory (Popov et al. 2016). Determination of anisotropy requires scanning direction parallel/vertical with foliation/lineation directions.

Calorimetric method

In addition to the TPS measurements, the calorimetric technique has been used in the site descriptive modelling in Forsmark to determine the heat capacity. The samples are placed in a temperature-controlled water bath long enough to stabilize. The calorimeter is filled with water to a defined level. The water in the calorimeter is stirred and the temperature logged. The sample is quickly moved from the bath into the calorimeter. The temperature rise of water is recorded during the equalization process (Adl-Zarrabi 2006).

4.4.3 Field measurements

The basis for *in situ* methods for measuring thermal properties is to add heat to a borehole and measure the temperature response in the rock. The *in situ* methods typically give a characteristic value for a larger volume compared to laboratory measurements. Field methods can be used as a supplement or replacement to laboratory methods.

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 larger scales (e.g. the simulation scale) are important in order to minimise these uncertainties. The appropriate scale for investigating variations in thermal properties in a rock volume is governed by the lithology, the modelling approach and the method used in the design of a final repository. In practice, the metre-scale is considered to be the most relevant, since small-scale variations are evened out at this scale, resulting in a considerable reduction in variance. At this scale, a rock type also includes rock occurrence and thus corresponds to the new definition of TRCs, see Section 5.4.3.

A review of various methods is presented in an action plan (Sundberg 2019), where suitable methods for field measurement during the construction and operational phase of the repository are suggested. In the action plan the following field methods are prioritized:

- DTS-Heat
- Multi probe method

DTS-Heat

Temperature measurements using fibre optic technology DTS (Distributed Temperature Sensing) have been used for many years in applications where there is a need to measure or monitor the temperature at many points over a long distance, e.g. along a power cable or monitoring the efficiency of a hydro-electric or mining dam. The technology has developed significantly in recent years for various purposes. With this technique, the temperature can be measured along a borehole. By integrating the fibre optic cable with a heating cable, heat can be applied in a similar manner to a single probe method. By using a specially designed inflatable sock, the cable can be pressed the wall of the borehole and water movements along the borehole can be reduced or eliminated. The thermal conductivity can thus be measured and evaluated simultaneously at different scales along the entire borehole. The method, here named DTS-H (Heat), has great potential and enables collection of a data base for conditioned modelling, both regarding property distributions and spatial correlation.

The methodology is described in Bense et al. (2016), and Patterson et al. (2017). The methodology has been tested by SKB in autumn 2017 in two boreholes in Forsmark (Johansson et al. 2022) but thermal conductivity has not been further evaluated. The method requires development to meet SKB's requirements regarding e.g. robustness and accuracy (Sundberg 2019).

Multi probe method

The multi probe method (Landström et al. 1979) is a development of the well-known (single) probe method. The theory is originally based on the infinite line source theory. The typical scale for single- or multi-probe measurements is in the range of 0.2–1 m. *In situ* measurements with the multi-probe method have been performed at the prototype repository in Äspö HRL (Sundberg and Gabrielsson 1999), in Forsmark (Sundberg et al. 2007) and in the Laxemar area (Mossmark and Sundberg 2007). The latter measurements were made at a larger scale, using a 2.4 m long heating probe.

Measurements with the multi-probe method can also be performed to analyze the thermal conductivity in different directions in anisotropic rocks. However, this demands simultaneous measurement of the temperature response in two directions, parallel and perpendicular to the anisotropy, and employment of a more advanced evaluation technique. In Forsmark measurements of anisotropy at different scales have been made (Sundberg et al. 2007).

4.4.4 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 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 an effective thermal conductivity. In a n-phase material, the effective thermal conductivity, λ_e, can be estimated from the following expression by iteration:

$$\lambda_e = \frac{1}{m}\left[\sum_{i=1}^{n} \frac{v_i}{(m-1)\cdot\lambda_e + \lambda_i}\right]^{-1} \quad (4\text{-}2)$$

where m is the dimensionality of the problem, λ_i the thermal conductivity of a grain, v_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 results are 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 a given type. This may be due to the limitations associated with the point-counting method used, which does not consider fully the presence of alteration products. In most cases these alteration products (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.

4.4.5 Density logging

A relationship between density and thermal conductivity for Ävrö granite in Laxemar/Simpevarp was found by Sundberg (2002). The thermal conductivity is inversely proportional to the density for felsic and intermediate igneous as well as for meta-igneous rocks. The reason for this is that the contribution of quartz content to the thermal conductivity dominates in relation to the contribution of density in these rock types.

The relationship has become well established and expressed mathematically (Sundberg 2003a, 2006, Wrafter et al. 2006). A similar relationship has also been observed for some of the rock types within the Forsmark site (Back et al. 2007). The observed relationship is also consistent with the more general results of theoretical calculations based on synthetic data with different mineral compositions of igneous rocks, presented in Sundberg et al. (2009); see Figure 4-5.

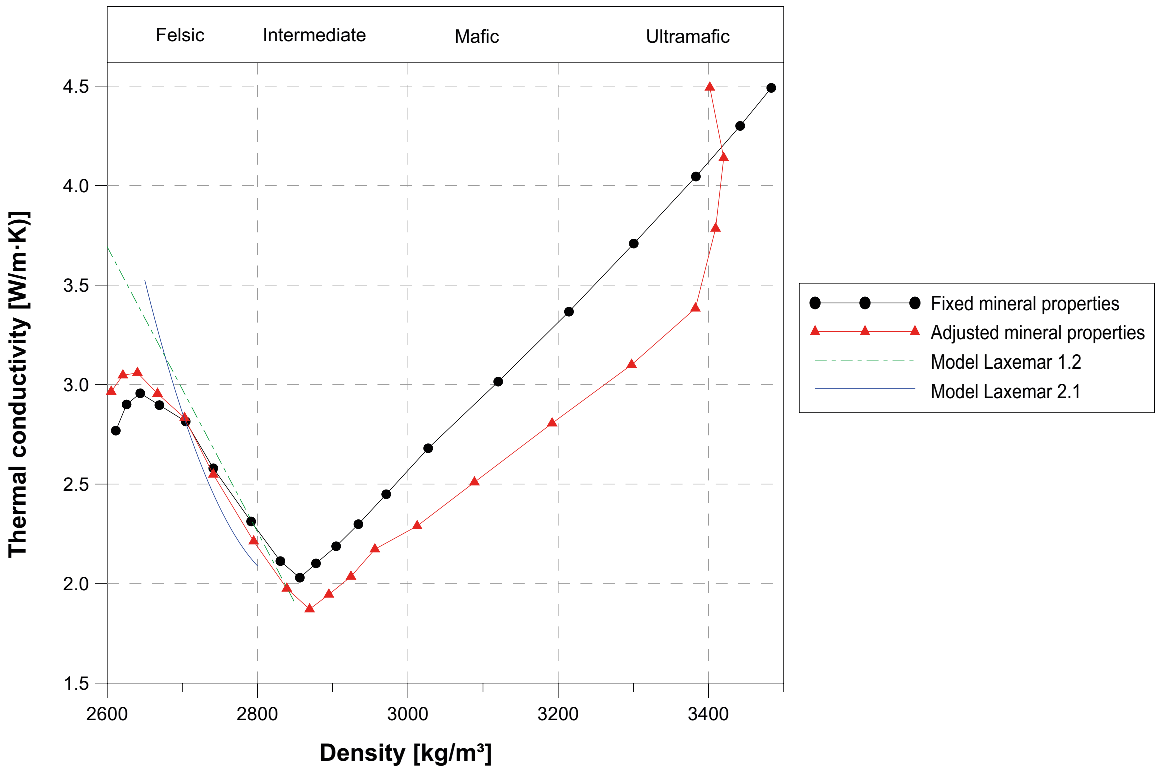

Figure 4-5. *Thermal conductivity versus density for synthetically defined data with different mineral compositions of igneous rocks (Sundberg et al. 2009).*

Density logging is thus a possible method to evaluate the spatial distribution and correlation structure of thermal properties for many rock types. Homogenous rock types have normally restricted ranges of density and may not show a clear correlation between these parameters. In Forsmark, thermal conductivity on rock types other than granite to tonalite (101051) and amphibolite (102017), have no obvious relationships with density according to Back et al. (2007). However, the density log may still be possible to use in order to create variograms to study the correlation structure; see Section 5.7.4.

4.4.6 Thermal conductivity versus heat capacity

It is reasonable to assume that there is a similar relationship between density and volumetric heat capacity as that found between density and thermal conductivity. Such a relationship can be seen in Sundberg (2003b), but it is weaker than that for thermal conductivity versus density. In Forsmark, such a relationship was found during the site descriptive modelling (Back et al. 2007); see Figure 4-6. This relationship is expected to be used in the thermal modelling and may be successively developed; see Section 5.11.

4.4.7 Thermal conductivity indications from 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 serve as a complement to other methods to estimate the thermal conductivity. Temperature loggings are also possible to use for evaluation of heat flow data.

4.4.8 Rock type versus thermal conductivity

Thermal transport properties can be correlated to rock type through the mineral composition (see also Section 4.3.1). Sundberg (1988) made calculations of thermal conductivity from mineralogical composition for about 4000 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.

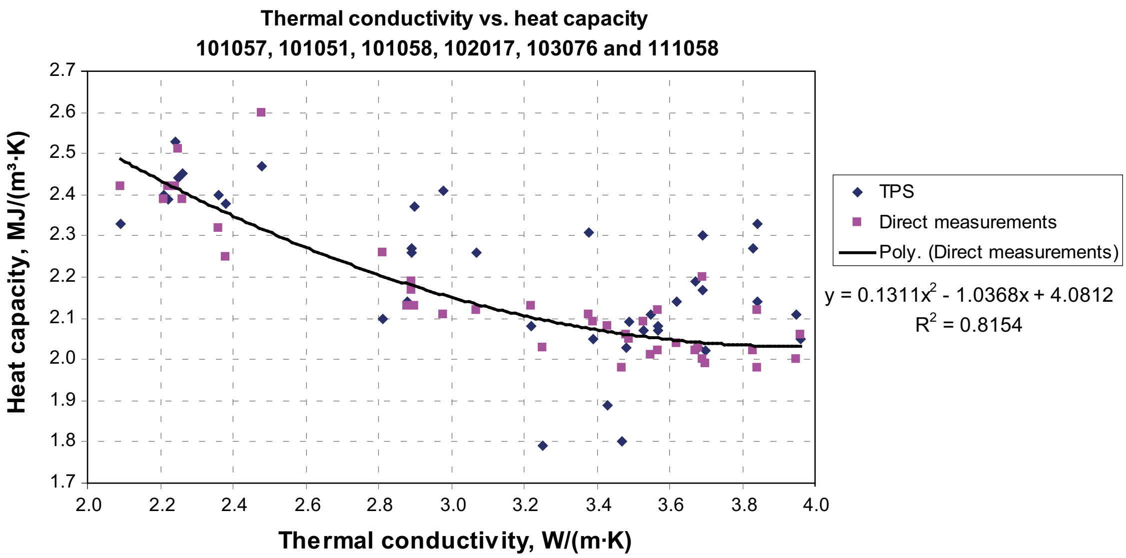

Figure 4-6. *Volumetric heat capacity versus thermal conductivity. The heat capacity is calculated from TPS determination and from calorimetric measurement. The second order relationship is based on calorimetric measurements only (Back et al. 2007).*

4.4.9 Comparison of methods for determining thermal conductivity

In Table 4-1, different thermal methods are compared. SKB have good experiences with the TPS method, described in Section 4.4.2. Continuous profiles of data along boreholes or borehole cores are important for evaluation of spatial dependence. Such profiles are possible to obtain with the TPS method but very expensive and consequently unrealistic. Another main drawback is the small measurement scale, both for normal and anisotropic measurements. The TPS method needs to be combined with density measurements to produce variograms.

One main advantage with the multi probe method (see Section 4.4.3) is the methods ability to measure thermal anisotropy at the decimetre scale.

The most suitable thermal method seems to be field measurements in cored boreholes with the DTS-Heat method (Section 4.4.3), which also is considered cost-effective in larger series of measurements (Sundberg 2019). The main uncertainty with the method seems to be that it is untested and requires development.

The main advantage with the density log is its ability to describe the spatial correlation structure of thermal conductivity.

Table 4-1. The ability of a selection of methods to meet the data needs for conditional modelling.

Type of data	Scale	Continuous profile in borehole	Quality for specified application	Modelling of thermal conductivity distribution	Modelling of variogram	Measurement of anisotropy
Laboratory data TPS	cm	No	High	Yes	No	Yes
Mineral data SCA	mm	No	Medium to High	Yes	No	No
Optical scanning	0.1–1 m larger	Yes	Medium to High	Yes	Yes	No
Field measurements DTS-Heat	0.1–1 m or larger	Yes	Medium to High	Yes	Yes	No
Field measurements Multi probe method	0.1–1 m	No	High	Yes	No	Yes
Density log	0.1–1 m or larger	Yes	Medium (?)	No[1]	Yes[2]	No

1) Only possible if a reliable relationship between thermal conductivity and density logging data can be determined, in combination with high quality of the density log.

2) High quality requires conditions in accordance with [1].

4.5 Determination of other thermal data

4.5.1 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 and depth, heat flow as well as versus thermal properties in the rock mass.

In Sweden, the geothermal gradient is in general about 0.01–0.015 °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 (Haenel and Hurter 2002). In a report on temperature conditions in the SKB study sites, the temperature gradients vary between 0.0095–0.0155 °C/m (Ahlbom et al. 1995).

4.5.2 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 significant. In Forsmark the internal heat production is calculated to approximately 2.7 $\mu W/m^3$ (Rath et al. 2019).

4.5.3 Thermal expansion of rock

The thermal linear expansion is measured on core samples in the laboratory. The tests and measurement methods are outlined in the SKB site investigation programme (SKB 2001). The results are used to calculate induced stress in the repository due to thermal load, which is of importance for the safety assessment (see further the rock mechanics methodology report, RMMM (Hakami et al. 2022)). Measurements made as part of the surface-based site investigations in Forsmark, showed no significant variation in thermal expansion coefficient due to rock type (Sundberg et al. 2005a).

4.6 Determination of boundary conditions

4.6.1 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 Section 2.1). 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 geology.

The geothermal heat flow is normally 35–70 mW/m^2. In the southern part of central Sweden, the heat flow can be somewhat augmented (Haenel and Hurter 2002). However, the reliability of 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 some cases measured, thermal conductivities. Uncertainties in the temperature logging result and the thermal conductivity estimation are therefore transferred into the heat flow determination.

4.6.2 Climate conditions at the surface

The actual climate conditions (Lindell et al. 1999) and prognoses for the future can be evaluated from climate databases and from studies by SKB (e.g. Brandefelt et al. 2013, Lord et al. 2019).

4.7 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 respect to the maximum temperature allowed on the bentonite buffer outside the canisters. 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.
- Deficiencies in the representativeness of the sampling.
- Insufficient number of samples and measurements.
- Variation due to potential anisotropy.

The three first types of uncertainty are associated with data uncertainties (Section 5.14.1) whereas the last one is a type of natural variability.

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.

5 Thermal modelling

5.1 Modelling approach

The approach for the thermal modelling is to model the spatial statistical structure of thermal properties and then perform stochastic simulation to produce realisations of the spatial distribution of thermal properties in the modelled rock volume. This requires data and the methodology is to some extent dependant on the type of data (scale and measurement technique), the amount of data, and the quality of the data. Insufficiencies in the data set can to some extent be compensated for by expert knowledge in the modelling process. In Forsmark expert knowledge is necessary since deposition tunnels will be aligned subparallel to the foliation; see Section 3.2.

The focus in the modelling is on the most important thermal transport property, the thermal conductivity. Heat capacity is not modelled explicitly by simulation. The reason is lack of data and that there is a constitutive relationship between thermal conductivity and heat capacity. Modelling with this correlation model is assumed to give a more correct outcome than utilizing standalone modelling of heat capacity; see Section 5.11.

The modelling is restricted to intact rock. Fracture zones will not be present close to the deposited canisters in the repository and the thermal influence of such zones on the local temperature field will therefore be small (Section 3.3). Consequently, fracture zones are not included in the thermal stochastic modelling approach. However, thermal properties of fracture zones can be considered during thermal dimensioning of the repository if required, i.e. if they define the boundary conditions.

Stochastic simulation is used in the modelling, which is a tool to perform uncertainty analysis or risk analysis. Several equally probable realisations are produced in the simulation, and the combined realisations represents the rock volume statistically. There is no prerequisite that data need to be normally (Gaussian) distributed. On the contrary, the methodology can handle data from any type of statistical distribution.

The stochastic simulation does not produce primary 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, but it can to some extent compensate for it. For example, prediction cannot produce correct values at locations where no measurements have been made, but by performing simulations it is possible to extract as much information as possible from the data set. Thus, simulation is a complement to data. It must be stressed that there does not exist one single realisation which is the most likely one; instead there is an infinite number of equally probable realisations. However, at a specific location, it is possible to predict the most likely value.

5.2 Outline of the methodology

The methodology for thermal modelling is presented in Figure 5-1. It consists of a procedure of ten steps:

1. Data collection.
2. Data interpretation.
3. Expert knowledge.
4. Statistical modelling of TRC lithology.
5. Statistical modelling of thermal properties.
6. Spatial thermal boundaries.
7. Stochastic simulation of TRC lithology.
8. Stochastic simulation of thermal properties.
9. Realisations of thermal properties.
10. Output to thermal dimensioning and evaluation of results.

The methodology, as outlined in Figure 5-1, is applied for each rock volume of interest, i.e. on sub-volumes of the repository. The approach was originally developed for modelling of a whole rock domain (Back et al. 2007) but it has now been adapted to include conditioned modelling of subvolumes.

Starting at the upper part of Figure 5-1, the thermal modelling work starts with data collection (1). The captured data is prepared and interpreted in the next step (2). This data interpretation step includes the choice of simulation scale, defining Thermal Rock Classes (TRCs), preparing lithological data, classifying lithological data as TRCs, preparing thermal data, and upscaling (change of support) of thermal data (if required). The result of these sub-steps is a defined set of TRCs and corresponding thermal data for each TRC, representing the simulation scale, i.e. the resolution of the thermal model.

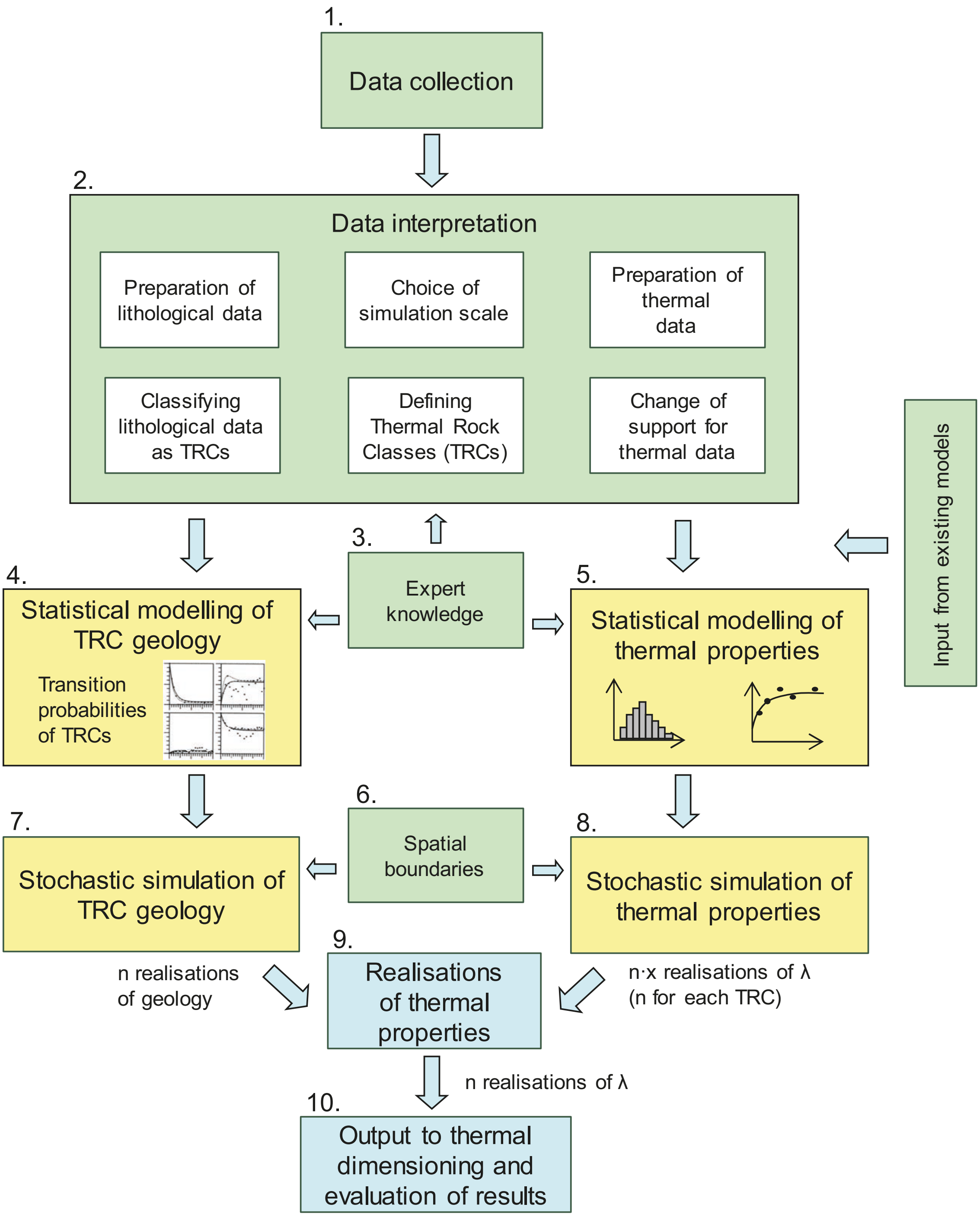

Figure 5-1. *Schematic description of the procedure for thermal modelling. The figure illustrates the workflow when applying the methodology, i.e. each box represents a certain work package. The outcome from the thermal modelling can be utilised as input to the thermal dimensioning of the repository in Figure 2-3.*

Expert knowledge and input from existing models (3), mainly geology, will influence the data interpretation step (2) as well as the modelling steps (4 to 10). For example, thermal models from the SDM can be used as a starting point, with new data being used to update and refine the models.

Expert knowledge (3) is of imperative importance, both during the data interpretation and the modelling steps. Such expert knowledge is utilized to bring the general knowledge down to the model level and to compensate for bias in the data. More explicitly, expert knowledge is applied for defining TRCs, for the statistical modelling of TRC lithology (4) and thermal properties (5). The statistical modelling of TRC lithology utilizes lithological data to construct models of the transition between different TRCs, thus describing the spatial statistical structure of each TRC. The result is a set of transition probability models that are used in the lithological simulation of TRCs (7). This simulation can be either conditional or unconditional. The intermediate result of this stochastic simulation is a number of realisations of TRC lithology, each one equally probable.

A prerequisite for the simulations is that the spatial boundaries have been defined (6). There are computational limitations on how large volume of rock can be simulated, and consequently, the modelling will have to be performed on subvolumes. This is also in accordance with application of the methodology on a successively evolving repository during the construction and operational phases.

Based on the thermal data, statistical thermal models are constructed for each TRC (5). A statistical thermal model consists of both a statistical distribution model and a variogram model. These are used in the stochastic simulation of thermal conductivity (8), either conditional or unconditional, and the result is a number of equally probable realisations of thermal conductivity for each TRC. Steps 4 and 7 can be carried out in parallel with steps 5 and 8 because they are independent.

In the next step (9), the realisations of TRCs (lithology) and thermal conductivity are merged, i.e. each realisation of geology is filled with simulated thermal conductivity values. The result 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. In addition, realisations of other thermal properties, primarily heat capacity, can be created in step 9 by applying a statistical relationship between thermal conductivity and heat capacity.

As the last step in the methodology (10), the realisations can be used directly in the thermal dimensioning, as described in Section 2.5. In addition, the modelling results can be analysed and presented in several ways, both regarding thermal and lithological properties in the modelled rock volume, the most obvious being predicted thermal conductivity values in subvolumes of rock. Other examples include 3D illustrations for visualization, histograms and statistical parameters (descriptive statistics), proportions of different TRCs, typical lengths and volumes of rock bodies, confidence intervals for specific properties, etc. If the result is desired at a scale different from the simulation scale, upscaling of the realisations can be performed to a desired appropriate scale.

Software considerations for the relevant steps are discussed in Back et al. (2022). Below, each step in the methodology is described in more detail. The chapter ends with three sections discussing how anisotropy is handled in the modelling, uncertainty in data and modelling, and model evaluation.

5.3 Step 1 – Data collection

Data capture is of fundamental importance for a successful thermal modelling. Both lithological data and thermal data are required. The thermal modelling can utilize previously collected lithological data and new data from boreholes and tunnels collected during the construction and operational phases of the repository.

In addition, thermal data needs to be captured for the thermal modelling. A thorough description of the different types of thermal data is given in Section 4.4. It is advantageous that data of thermal conductivity represent that same scale as the simulation scale, i.e. the resolution of the thermal model, since this will facilitate the modelling significantly. A simulation scale of around 1 m is recommended; see Part 2 (Chapter 2 in Back et al. 2022), which means that thermal data should represent the same scale. Field measurements in pilot boreholes at this scale is therefore advantageous.

Thermal data from pilot boreholes should cover as large parts of the boreholes as possible. There are several reasons for this:

- Large data sets will facilitate conditional simulation in the vicinity of the boreholes.
- Large data sets, representing relatively short distances, are required in order to calculate reliable variograms for modelling of the correlation structure of thermal conductivity for each TRC.
- Similarly, large data sets will increase the reliability of histograms.

Data requirements are further discussed in Chapter 6.

5.4 Step 2 – Data interpretation

5.4.1 Procedure

The data interpretation step is a bridge between data collection and modelling. The objective is to prepare and interpret data in such a way that it can be utilized in the modelling work performed in subsequent steps. It is in the data interpretation step the important concept of TRC, Thermal Rock Classes, is introduced in order to facilitate the thermal modelling. The data interpretation step consists of six sub-steps:

- Choice of simulation scale.
- Defining Thermal Rock Classes (TRCs).
- Preparing lithological data.
- Classifying lithological data as TRCs.
- Preparing thermal data.
- Change of support for thermal data.

Each step is described below.

5.4.2 Choice of simulation scale

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, i.e. the resolution of the simulated rock volume. The simulation volume is defined as all the grid cells in a realisation. Background information on the choice of simulation scale is presented in Part 2 (Chapter 2 in Back et al. 2022).

The following are considered when choosing the simulation scale:

- Preferable, the simulation scale should be equal to the scale (support) of measurements, i.e. the data scale. This will make change of support (Section 5.4.7) unnecessary.
- The simulation scale must be sufficiently small to reflect small-scale variations in lithology and thermal properties that may be of importance. Typical dimensions of the important rock types, both dominating in terms of volume and subordinate, should be considered.
- The simulation scale must be sufficiently large so that the number of grid cells does not become too large. Due to limitations in computer capacity, software, and time, there is a practical limit for the number of grid cells in a simulation volume.
- The data requirements of the end user should also be considered when the simulation scale is defined.

If the data scale is small, a change of support may be required, according to Section 5.4.7; see Figure 5-2. If possible, this should be avoided since upscaling is a source of uncertainty in the modelling. One way to avoid this is to increase the measurement scale by field measurements, as illustrated in the figure.

In Part 2 (Back et al. 2022) it is concluded that a simulation scale of at least 0.5 m, and preferable 1 m or more, is desirable.

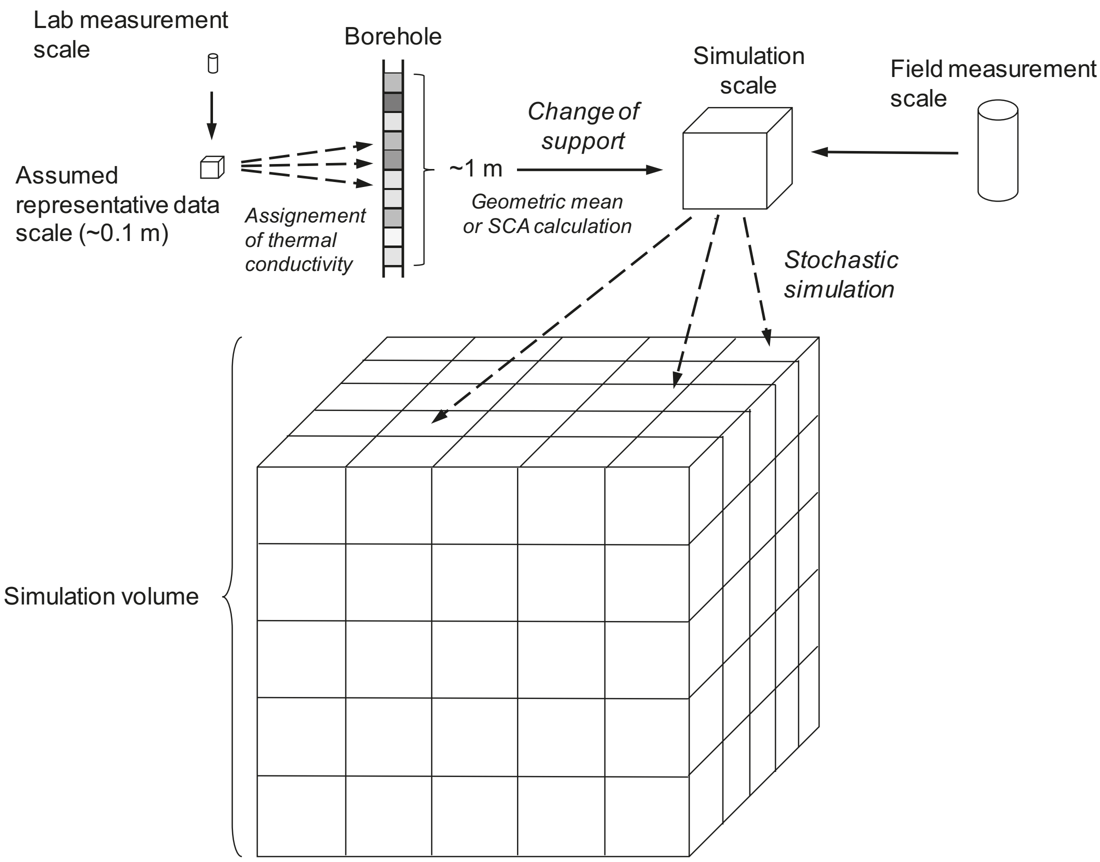

Figure 5-2. *Illustration of sample support, change of support, simulation scale, and simulation volume. Note the different approaches depending on if data is available in lab measurement scale or in field measurement scale.*

5.4.3 Defining Thermal Rock Classes (TRCs)

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 rock types directly is that the number of rock types present usually exceeds the number of classes that can be handled in the stochastic simulation of TRC lithology (step 7). By defining TRCs, the complexity of the simulations can be kept at a reasonable level. The TRCs imply a slightly rougher classification than rock types but the TRCs are sufficiently detailed to handle the description of thermal conductivity.

The way TRCs are defined has changed compared to the Site Descriptive Modelling. Background on the changed definition of TRCs, for application during the construction and operational phases of the repository, is presented in Part 2 (Chapter 3 in Back et al. 2022). A conclusion is that it is possible to use the entity *rock type* in Boremap as a basis for defining TRCs, and at the same time include *rock occurrences* that will exist within the simulation scale in boreholes and tunnels. Thus, the TRCs are coupled to a defined scale, preferably the selected simulation scale.

The following definition is suggested for TRCs for rock in domain RFM029:

- TRC-57, comprising rock types 101057 and 101058, and all rock occurrences.
- TRC-51, comprising 101051 and all rock occurrences.
- TRC-61, comprising 101061 and 111058, and all rock occurrences.
- TRC-17, comprising 102017 and 101033, and all rock occurrences.

This way of defining TRCs has advantageous features for the thermal modelling. One is that Boremap data of rock type can be used directly to assign TRCs to data at the simulation scale (suggested scale is 1 m). In addition, rock occurrence in Boremap can also be used directly. This simplifies the process of defining TRCs, and it is in accordance with the geologists' classification of rock. The approach was tested (see Part 2) by Back et al. (2022) and considered successful. It is therefore the recommended approach for the construction and operational phases of the repository.

Statistical inhomogeneity may require subdivision of TRCs to improve the thermal modelling; see Sections 5.7.2 and 5.7.5. This may be enhanced by interdisciplinary cooperation; see Section 3.4.

5.4.4 Preparing lithological data

Procedure

The lithological information mainly consists of data from cored boreholes and tunnel mapping. Systematic sequential pilot borehole drilling is planned in accordance with the layout of main, transport and deposition tunnels. An overview is given in Figure 3-1.

However, the representativeness of borehole data will depend on how the directions of the boreholes are decided. If boreholes are directed with the objective to avoid certain lithological features, such as low-conductive rock occurrences, this may result in bias in the lithological data. Such a data set does not constitute a random sample and consequently, modelling based on such data cannot be assumed to give completely representative simulation results. Therefore, a method to adjust for bias in lithological data may be required in order to avoid systematic errors in the modelling. This issue is further discussed in Section 5.14 and in Part 2 (Back et al. 2022).

The lithological data should be complemented with geological expert knowledge when required (Figure 5-1), see also Section 3.4. The data need to be processed before it can be utilised in the simulations. The aim of the data processing is to assign TRCs to the data, at a resolution that matches the simulation scale. This is a two-step procedure. First, the lithological data must be adjusted to the relevant scale. The resolution in Boremap data is 1 cm, but the data that will be used in the simulations should match the simulation scale, i.e. the size of a grid cell. The next step is to assign TRCs to the processed lithological data (Section 5.4.5). These two steps are overlapping and performed simultaneously.

Both rock type and rock occurrence in Boremap are considered during data preparation and definition of TRCs, but a problem is how to handle rock occurrences with an apparent thickness less than the cell size. How this is performed is described below.

Handling of rock occurrences

The approach for handling rock occurrences is to use Boremap data directly. The principle is to define a TRC as a fusion of rock occurrences and the surrounding rock, i.e. according to the classification in Boremap. The objective is to consider the effect of rock occurrences at a scale smaller than the grid cell, which could be important when a simulation scale of 0.5 m or larger is used. In this way, the thermal properties of a TRC will be a mixture of the rock types occurring at the simulation scale or smaller. Not only the lithology is fused but also the statistical distributions of thermal conductivity for the different rocks. In Part 2 (Chapter 3 in Back et al. 2022), the approach was tested out on Boremap data from four boreholes.

The data preparation must consider the inclination and bearing of boreholes, so that representative statistics of the spatial structure of TRCs can be properly developed (Section 5.6) and biased statistics avoided (Section 5.14). In Back et al. (2022), it is described how bias due to boreholes deviating from anisotropy directions can be corrected for by transformation of the model domain to anisotropy directions. However, there may still be bias to be corrected for, since more information will by necessity be available from the vertical or sub-vertical directions than the horizontal directions, especially during the initial stages of repository construction and operation. The bias is expected to decrease when the number of horizontal boreholes increases, as the operation of the repository progresses. It is suggested that expert elicitation is explored for improving the information and decreasing bias (Section 5.5).

Considerations for conditional simulation

For conditional simulation, there are some data requirements that should be met to make prediction more reliable:

- The conditioning lithological data set should be as large as possible.
- The conditioning lithological data should be located as close as possible to the rock volume where prediction is desired.
- Boreholes with conditioning data should preferable be located close to each other. Different borehole directions could also be advantageous.

These requirements are expected to be met when a set of pilot boreholes (some 5 to 10) for deposition tunnels are available (constituting the foreseen annual batch). The associated data should provide a good platform for conditioned predictions.

5.4.5 Classifying lithological data as TRCs

In the previous step, lithological data are selected and prepared. The next step is to classify this data as TRCs. The classification is performed according to the definition of the TRCs, such as in the example for rock domain RFM029 in Section 5.4.3. The principle is simple when data from boreholes are used:

- The Boremap data are divided into sections of the same length as the resolution of the simulations, i.e. the simulation scale.
- Each section is assigned a TRC based on rock type in Boremap.

The result of the classification is a data set of TRC lithology. This data set will match the simulation scale, and the thermal data set prepared in Section 5.4.6 (or after upscaling in Section 5.4.7 if required).

5.4.6 Preparing thermal data

Types of thermal data

The different types of thermal conductivity data are presented in detail in Section 4.4. The main suggested data types during the construction and operational phases are (see Table 4-1):

- TPS measurement in the laboratory.
- Optical scanning of cores in the laboratory.
- Continuous field measurements in boreholes at 1 m scales, by the suggested DTS-Heat method.
- Field measurement with the multi probe method enabling measurement of anisotropy in the decimetre scale.
- Density logging data combined with a determined statistical correlation between thermal conductivity and density.
- Calculated thermal conductivity data from mineral compositions, by the self-consistent approximation (SCA) method.

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, but also by optical scanning. These two types of data are the main source of information for defining histograms for TRCs (Section 5.7.3). Thermal data requirements are further described and evaluated in Section 6.2.

Thermal conductivity data are used at two different occasions in the thermal modelling methodology:

- Statistical modelling of thermal properties (Section 5.7), as a basis for the subsequent simulations.
- Conditioning during conditional simulation (Section 5.10).

These different uses are described below. The data are generally the same for the two occasions, although this is not entirely necessary. In principle, small scale data could be used for the statistical modelling of thermal properties, whereas conditioning data could come from field measurements at a larger scale. This would require upscaling of the thermal models but not of the conditioning data.

Data for statistical modelling of thermal properties

As for lithological data, a data preparation step is required also for thermal data, as a preparation for the statistical modelling of thermal properties in step 5 (Section 5.7). The data preparation consists of error checking and, if required, declustering. Checking of errors and poor representativeness in the data is required because of human errors but more importantly because of the difficulty in classifying rock samples of varying composition and alteration into defined rock classes (this is mainly an issue when using small scale data). Outliers in the data set are good indicators of such problems.

Information about spatial variability requires large data sets and preferably, measurements of thermal conductivity should be used, if the data set is large enough. The use of the DTS-Heat method provides long continuous profiles of thermal conductivity and is suitable to use for spatial variability analyse. In addition, the DTS-Heat method may provide data that matches the simulation scale and can be used directly to enhance the modelling of spatial variability, if proven successful in providing thermal conductivity data.

If the DTS-Heat method cannot be used, information about spatial correlation must be acquired in a different way. A recommendation is to use the optical scanning method. Density logging data may be used if no other data is available, at least for those rock types where large variability in thermal properties and where a relationship exists between density and thermal conductivity.

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 volume. This is an aspect to consider in Forsmark for samples of granite and granodiorite (TPS data).

The requirements on thermal data for statistical modelling of thermal properties 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 5.4.7.
- It is desirable that the thermal data set is large 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 5.5.

Thermal data for conditioning

Conditioning data are data at specific grid cells that have fixed values during the stochastic conditional simulation. Such data will influence the simulated values of grid cells in their vicinity. Data used for conditioning should match the simulation scale. Upscaling of data for conditioning should be avoided, if possible. It is a source of additional uncertainty because the conditioning data will have a significant impact on the predicted thermal conductivity in the rock volume. However, if required, upscaling could be performed; see Section 5.4.7.

Contrary to the objective of statistical modelling of thermal properties (see above), declustering should not be performed on conditioning data. On the contrary, conditioning data appearing in clusters is advantageous because it will make prediction more reliable in the vicinity of the clusters.

The requirements of thermal data for conditioning are:

- 3D coordinates must be available for each data point.
- Conditioning data should be of high quality because it will have significant impact on predicted thermal conductivity.
- The conditioning data set should be as large as possible because this will improve the reliability of predictions made.
- Conditioning data points should, if possible be spatially located closer to each other than the established correlation length (range). This will significantly increase the reliability of predictions.

- The conditioning data should be located as close as possible to the rock volume where prediction is desired.
- Clustering of conditioning data does not constitute a problem, rather an advantage.

Conditioning data are only a matter to consider in conditional simulation, not if the simulation is unconditional.

5.4.7 Change of support for thermal data

The support of a measurement is the volume, shape and orientation that the data value represents (Starks 1986), in this case thermal data. A change of support, or upscaling, is only required when the measurement support is significantly smaller than the simulation scale, i.e. smaller than the grid cells in the simulation volume; see Figure 5-2. Change of support is not an issue if thermal data are available in the suggested 1 m simulation scale. However, a change of support may be required when different types of data need to be combined, such as laboratory measurements and field measurements representing different scales. Note that it is only thermal data that are subject to change of support, and only if required. Lithological data are adjusted to the simulation scale in the data preparation described in Section 5.4.4.

Upscaling of thermal data results in a changed shape of the histogram; the variance is reduced, and the mean is slightly affected. In addition, upscaling will affect the spatial correlation structure, i.e. the variograms. However, upscaling is also a source of uncertainty and should therefore be avoided if possible. Upscaling is especially troublesome when conditional simulation is used because it will add an uncertainty component to the conditioning data, which in turn are used as a basis for simulated values in surrounding rock. The best way to avoid the support problem is to use data that have the same size as the grid cells in the simulations, i.e. the simulation scale (Isaaks and Srivastava 1989).

Upscaling requires a simple method that can be used simultaneously with the data preparation. It is performed by (Figure 5-2):

1. Assigning thermal conductivity (randomly) directly to Boremap data at a small scale, approximately 0.1 metre.
2. Dividing the borehole data in sections with a length corresponding to the simulation scale (about 1 m).
3. Calculating thermal conductivity for each section by the use of geometrical mean or the SCA approach (see Section 4.4.4).

This method for upscaling was tested in Back et al. (2022). It will result in thermal properties at the desired simulation scale, thus eliminating the need of using stochastic simulation for the purpose of upscaling.

5.5 Step 3 – Expert knowledge and input from existing models

In Forsmark, the hard data discussed in Sections 5.4.4 and 5.4.6 will not sufficient. Expert knowledge will be required as a complement in order to complete the statistical modelling of TRC lithology and thermal properties; see Section 5.6 and Section 5.7 respectively. The validity of hard data from boreholes and tunnels depends on the degree of lithological homogeneity. The statistical models and correlation models of TRCs must be realistic, which demands 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, correlation structure, and anisotropy, are necessary inputs. Expert knowledge is also required when the lithology in different boreholes and tunnels is statistically different (an indication of statistical heterogeneity). Geological expert knowledge must be used to assess the representativeness of the different data sets, and if and how the rock volume should be divided into more statistically homogeneous subvolumes that can be modelled separately; see Section 5.6. In Part 2 (Back et al. 2022), it is suggested that expert elicitation is explored for improving the information and decreasing bias regarding spatial statistical properties such as lengths, orientations and proportions of lithological units. It is suggested that the SHELF method or a similar method is considered to use for expert elicitation.

The statistical models of thermal properties (statistical distribution and variogram) require 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 directions where data are sparse. In addition, expert knowledge is needed to distinguish sub-TRCs in cases of non-homogeneous statistical thermal properties of a TRC; see Section 5.7.5.

The statistical models of thermal properties will be based on all available data, not necessarily only data from the simulation volume. This implies that expert judgement must be applied to assess whether data acquired from outside the simulation volume will influence the modelling, especially whether a bias is introduced or not. This situation may occur if data are sparse, and especially if the thermal conductivity exhibit large-scale spatial variability (trends over long distances).

The thermal modelling should aim at reducing the need of expert judgement. One way of doing so is to increase the amount of appropriate data from the simulation volume, especially for conditional simulation. This will reduce the uncertainty.

5.6 Step 4 – Statistical modelling of TRC lithology

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

1. Calculate values of a spatial statistic (e.g. variogram) at regularly spaced lags (separation vectors).
2. Fit a mathematical function (e.g. spherical or exponential) to the experimental variogram.
3. Implement selected estimation (e.g. Kriging) or simulation (e.g. sequential simulation, simulated annealing) procedures of choice.

Geological expert knowledge does not necessarily enter directly into this procedure. Therefore, another approach is suggested to model spatial conditions: Markov chain analysis. In this approach, the transitional trends between geological materials are analysed. Spatial modelling using Markov chain analysis can utilize geological expert knowledge and makes it possible to more directly and explicitly consider factors with geological implications, such as:

- volumetric proportions of TRCs,
- 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.

Motives for using Markov Chains are further discussed in Part 2 (Chapter 4 in Back et al. 2022), as well as other possible options.

The modelling consists of calculating transition probabilities followed by expert adjustments based on geological interpretations; see Section 5.5. Hard data input consists of Boremap data reclassified as TRCs (Section 5.4.3). 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 5-3, with four TRCs, i.e. 16 possible transitions from one TRC to another (16 graphs). 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. Software is required for creating the transition probability plots in Figure 5-3. One such software is T-PROGS (Transition PRObability GeoStatistics) (Carle 1999, GMS 2019). More information on transition probabilities and Markov chains are provided in Part 2 (Chapter 4 in Back et al. 2022).

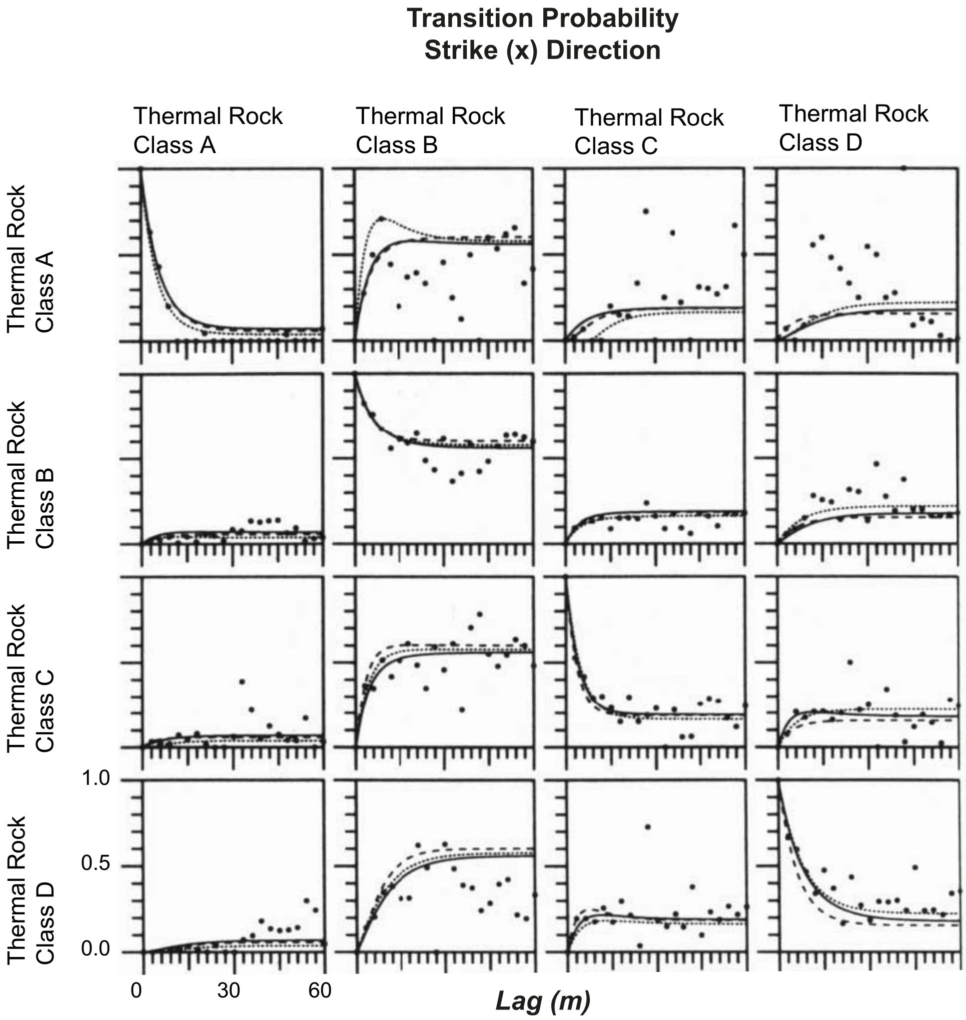

Figure 5-3. *Principle of transition probabilities using Markov chains for 1D simulation (after Carle and Fogg 1997). The graphs present the probability of transition from one thermal rock class to another when moving from one cell to the next in the strike direction.*

Statistical homogeneity is assumed throughout the modelling volume, which is a central assumption in geostatistics. Incorrectly assuming statistical homogeneity of the geology[3] may lead to problems of reproducing the true heterogeneity of the modelled rock volume. In Forsmark, differences in the composition of the rock may violate this assumption in some circumstances, especially if the modelled volume is large. Therefore, statistical heterogeneity[4] requires special attention. A solution is to divide the rock volume into smaller subvolumes, so that each subvolume can be assumed to be statistically homogeneous. The spatial statistical structure of TRCs is then modelled separately for each subvolume and stochastic simulation of the geology (Section 5.9) is also performed separately for each subvolume. The combined realisations of all subvolumes are then used to represent the whole rock volume, consideration being taken of the relative volumetric proportion of each subvolume. For smaller rock volumes, statistical homogeneity can often be assumed, making the modelling easier.

Anisotropy in the lithology requires special attention. For example, it may be necessary to use a local coordinate system during the modelling, with axes oriented parallel and perpendicular to the principal axes of anisotropy (with following back-transformation). Expert judgement will be necessary since important data is expected from pilot holes aligned parallel to subparallel to the foliation, see Section 3.2.

[3] The geology is modelled statistically by transition probabilities, according to Figure 3.3.

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

5.7 Step 5 – Statistical modelling of thermal properties

5.7.1 Procedure

The objective of this step is to create spatial statistical thermal models describing the statistics and the spatial correlation structure of thermal conductivity for each TRC. 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).

These three steps are described below. Last, an approach of using sub-TRCs are discussed, for managing situations when thermal conductivity is not statistically homogeneous within a TRC.

5.7.2 Trend analysis

There may be large spatial trends in space (non-stationarity[5]) 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 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.

It requires a lot of data to perform a reliable quantitative trend analysis for a large rock volume. This is not an option when data are sparse, but it is suggested that at least 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 and tunnels. Density log data may also be an option.

If large spatial trends or statistical heterogeneity are detected, it may be justified to model the rock type as two separate TRCs; see Section 5.4.3. Alternatively, the data set of a TRC could be subdivided into separate populations and spatial statistical thermal models could be developed for each population (sub-TRC; see Section 5.7.5). 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.

5.7.3 Fitting a distribution model

The next step is to fit a distribution model to the histogram of thermal conductivity data. Alternative approaches for this step are:

1. Use the histogram directly as a model, without fitting of a mathematical 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, e.g. a normal distribution or a lognormal distribution.

The first approach is used when data as such 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.

One problem when data are sparse is how to model the tails of the histogram where there are no or very few data. The following principles are proposed 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 (regardless of the type of measurement).
2. Since the number of data is limited it can be assumed that values outside the measured range of the data exist in the rock volume. Therefore, it is reasonable to extend the interval range, depending on

[5] See the geostatistical literature for definitions of different types of stationarity, e.g. Chilès and Delfiner (1999) and Journel and Huijbregts (1978).

the number of data and the appearance/shape of the histogram. This is performed based on statistical principles[6].

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" implying mineral compositions which produce the lowest thermal conductivities).

Generally, more data are required to properly model a TRC when data exhibit large variability. The variability in data depend on:

1. The variability of thermal conductivity in the TRC.
2. The type of measurement used to acquire the data.
3. The scale (support) of the measurements.

The first source of variability cannot be reduced. The latter two sources of variability result from the measurement technique. High quality measurements reduce the second type of variability. The third type is reduced by measurements performed at a larger scale. Thus, the lowest amount of data is required for TRCs with low variability and where measurements are performed with high quality at a large scale. Possibly, the DTS-Heat method could supply such data, but this needs to be further developed and tested.

The distribution model of a TRC should reflect all rock types belonging to that TRC. Therefore, it must be considered that there are different amounts of data for the different rock types in a TRC. If measurements are performed at a larger scale, some of these issues can be avoided.

As quality control, the distribution models for different TRCs should be checked against other types of data, if available. For example, a distribution model derived from TPS measurements should be compared to SCA-calculated data. The importance of such a test is accentuated when data sets are small, when several rock types are included in the rock type name, or when bias is suspected.

5.7.4 Variogram modelling

The variogram modelling (structural analysis) is an important step in the thermal modelling. It will dictate how the variance is reduced when the scale increases, which affects the thermal conductivity distribution at different scales. Even more, the variogram model will determine how far from a borehole that reasonable predictions of thermal conductivity can be made within a TRC. The range (or correlation length) of the variogram model sets an upper limit of this distance (Figure 5-4). At larger distances, the predicted thermal conductivity will not be correlated with the conditioning data in the borehole. In this way, the variogram model will have a central role in the prediction.

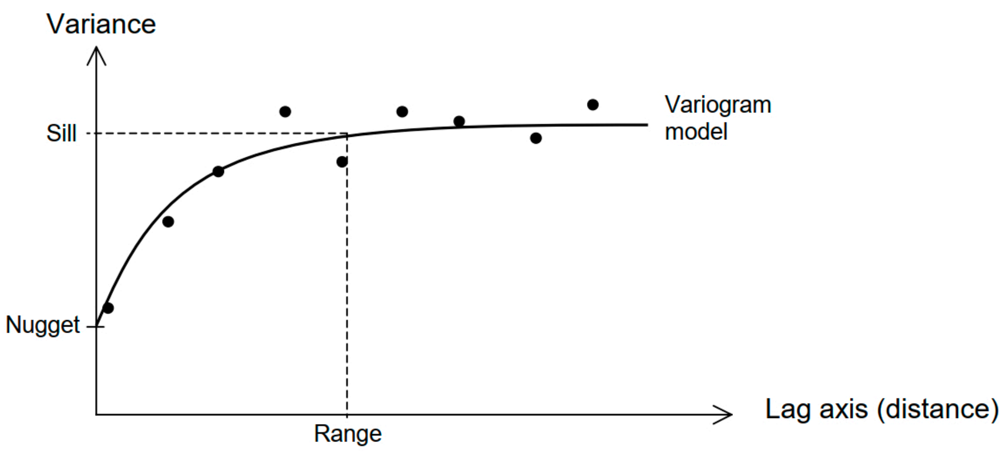

Figure 5-4. *Illustration of a variogram model with sill, nugget and range (Back 2001).*

[6] 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 model should characterises the main features of the spatial variability (correlation structure). 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). A set of principles are suggested for the variogram modelling:

1. Base the variogram model on the dominant rock type in each TRC.
2. Base the nugget of the variogram on the most reliable data. Use a low value when the nugget is uncertain; a high nugget may underestimate the variability in the thermal conductivity distribution after upscaling.
3. Estimate the range (correlation length) based on a sufficiently large set of thermal conductivity measurements, if possible. If the data set is small, other information correlated with thermal conductivity could be used instead or as a complement, such as density logging data, if a correlation can be determined.
4. Use omni-directional variogram models, if thermal data do not suggest otherwise, i.e. calculated 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 variability of the thermal conductivity distribution, i.e. a conservative approach[7].

The variogram model is always associated with modelling uncertainty, which is an important uncertainty to consider in the methodology; see Section 5.14.2. 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.

For some rock types, complex spatial patterns can be expected. 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 or tunnels. Such problems cannot be solved by nested variograms (see the section above on 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 5.13). 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 probably sufficient.

5.7.5 Sub-TRCs

Spatial statistical analysis of thermal conductivity could indicate that all TRCs are not statistically homogeneous. If this is the case or not will be obvious when histograms of calculated thermal conductivity values are compared for different boreholes. In addition, the spatial correlation structure (variograms) may also differ. In cases where this heterogeneity is believed to have significant effects, the TRC can been divided into sub-TRCs from a thermal point of view. The division should be made so that each sub-TRC is statistically homogeneous. Since the geological borehole mapping does not distinguish between these different types (it is a thermal difference), this issue cannot be dealt with in the lithological simulations by increasing the number of TRCs. Instead, the solution is to develop different statistical thermal models (Section 5.7) for each sub-TRC, representing each sub-population of thermal conductivity.

After the sub-TRCs are defined, and a statistical thermal model are assigned to each sub-TRC, then stochastic thermal simulation is performed separately for each one. The number of realisations produced during simulation for each sub-TRC corresponds to the proportion of the total TRC that the individual sub-TRCs is estimated to occupy.

After performed simulation, all realisations for all sub-TRCs are combined to form a single set of thermal realisations that represents the whole TRC of interest.

[7] 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 (or high) values occur in clusters, which affects the thermal conductivity distribution after upscaling.

5.8 Step 6 – Spatial thermal boundaries

The spatial boundaries for the stochastic simulations are defined in this step. These boundaries are defining the modelled rock volume and are intimately coupled to a successively evolving repository. Each sub-volume that is modelled will have its own spatial boundaries.

There are size limitations in the simulation tools that will influence the choice of spatial boundaries for the simulations. These limitations have been evaluated in Back et al. (2022). Computing time for the simulations puts restrictions on the size of the simulation volume. A reasonable size of the simulation volume is in the order of 1 000 000 m^3, when the resolution is 1 m (approximately a volume containing five deposition tunnels). See also Section 5.4.2 on this issue.

The spatial boundaries also include the developed underground openings (tunnels and deposition holes) during the construction and operational phases. These are included and handled in a simple way, primarily by masking of the resulting realisations (step 9). Thus, such openings do not constitute a problem for the stochastic simulation. The results from the modelling can be checked when a tunnel is mapped.

5.9 Step 7 – Stochastic simulation of TRC lithology

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); see background information in Part 2 (Chapter 4 in Back et al. 2022). 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 can be used for these simulations. The software utilizes transition probabilities based on both Markov chains and indicator simulation to create 3D realisations. Both conditional and unconditional simulation can be performed, and both approaches where used during the site descriptive modelling. Additional background information on simulation of TRC lithology is given in Part 2 (Back et al. 2022).

First, a model is built of the spatial statistical structure of the TRCs, according to Section 5.6. 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, which means that it is important that the data underlying the model really represent the simulation volume. 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 volume. An example of a 2D-realisation is illustrated in Figure 5-5.

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 (expert judgement). Otherwise, modifications of the spatial statistical structure of TRCs may be required. Revision of the TRCs (Section 5.4.3) may also be needed.

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

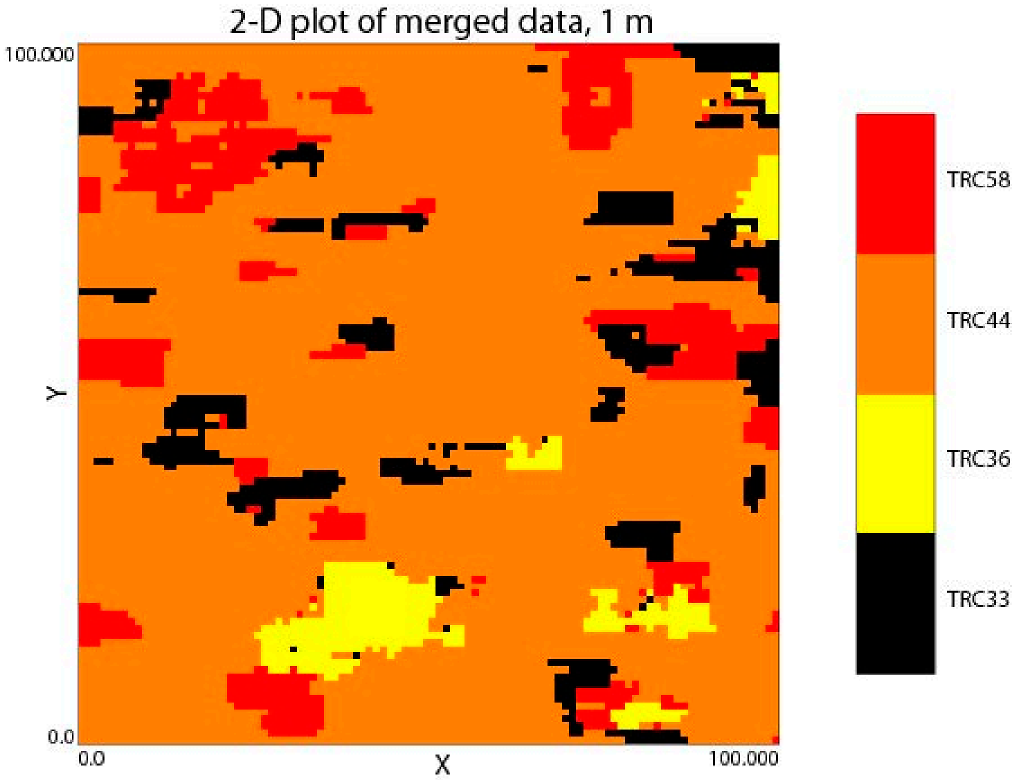

Figure 5-5. *Illustration of a 2D slice from one 3D realisation of TRCs.*

5.10 Step 8 – Stochastic simulation of thermal properties

Sequential Gaussian Simulation (SGS) is used for simulating the thermal conductivity within each TRC; see background information in Part 2 (Chapter 5 in Back et al. 2022). Consequently, one simulation is performed for each TRC. The basis for the SGS is the distribution model and the variogram model (Section 5.7). 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. Thermal conductivity follows other statistical distributions. However, this is of limited practical importance because the simulation software is designed to perform normal score 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 are not further discussed.

Both conditional and unconditional simulation can be performed. For prediction purposes during the construction and operational phases of the repository, conditional simulation is suggested.

An important aspect to consider in the simulation is the inclusion and 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 so-called lithotype (Deutsch and Journel 1998). Examples of such features are 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). The number of realisations must be decided based on the objective of the simulation and the size of the simulation volume. The number of realisations must be sufficiently large to produce a stable thermal conductivity distribution, i.e. the statistics of all realisations combined should not change significantly if more realisations are added.

5.11 Step 9 – Realisations of thermal properties

In this step, 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 5-6 in 2D. 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.

In addition, realisations of heat capacity could be created in this step. As indicated in Section 4.4.6, there is a relationship between thermal conductivity and heat capacity in Forsmark. By applying this relationship, realisations of heat capacity can be created from the thermal conductivity realisations; see Sundberg et al. (2008b) and Back et al. (2007).

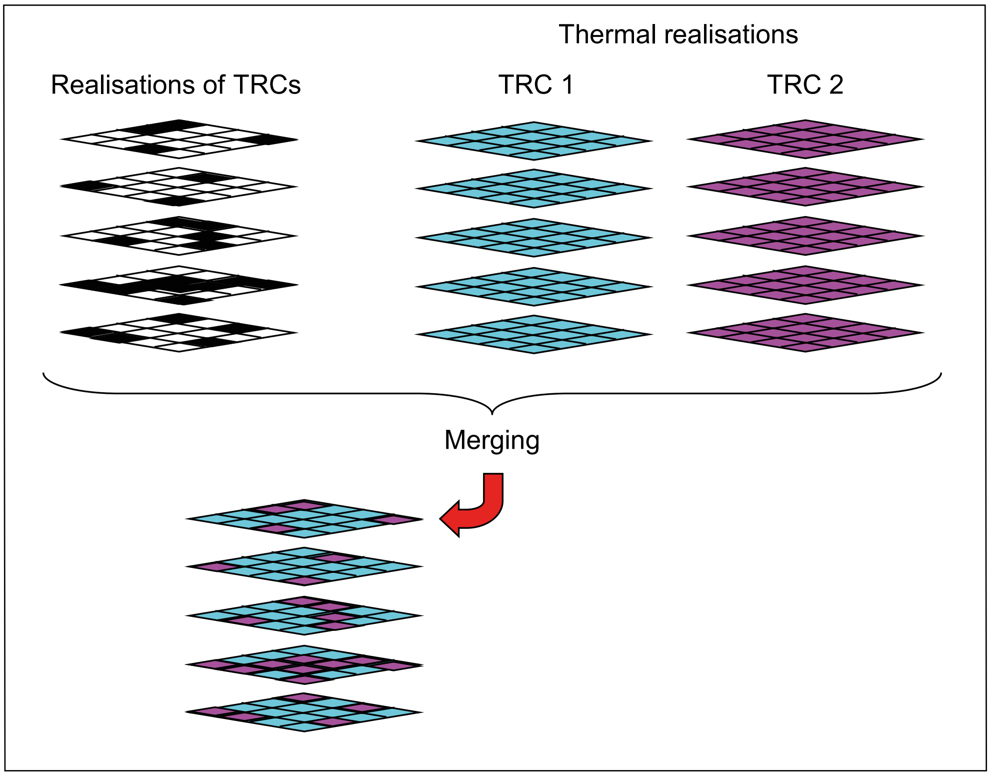

Figure 5-6. *Schematic description of the merging of TRC realisations (geology) and thermal realisations for two TRCs (2D realisations). The geological realisations control from which TRC a thermal conductivity value is selected. The same principle applies to 3D-realisations and when there are additional TRCs. The spatial variability of thermal conductivity within each TRC is not illustrated in the figure.*

5.12 Step 10 – Evaluation of results

5.21.1 Upscaling of simulation results

The result of the thermal modelling is a set of equally likely realisations of both lithology and thermal conductivity. The modelling results can be analysed and presented in different ways, primarily regarding thermal properties in the model volume (Section 5.12.2). In addition, the ranking procedure in Section 2.5 could be applied on the realisations, even without subsequent numerical modelling (Section 5.12.3). Also, lithological properties can to some extent be analysed (Section 5.12.4).

Upscaling of the simulation results can be performed if results are required at a different scale than the simulation scale. If required, such upscaling can also be used to study how the result varies with scale, plotted on a graph; see e.g. Back (2007). This could be imperative when viewing the model volume from different perspectives: small scale, canister scale, and repository scale. The upscaling is performed with the SCA approach (see Section 4.4.4).

5.12.2 Thermal properties in the model volume

For the objective of **description**, thermal properties can, for example, be presented as:

- Histograms of thermal conductivity representing the rock volume of interest. Such histograms can be presented for different scales, as illustrated by e.g. Back et al. (2007).
- Statistical parameters of the thermal conductivity distribution, such as the mean and percentiles (the 1-percentile representing the lower 1 % tail of the distribution); see e.g. Back et al. (2007).
- Quantified uncertainties in statistical parameters of the thermal conductivity distribution, e.g. expressed as confidence intervals. These can be calculated based on the variability in the realisations produced by simulation; see Back et al. (2007).
- Percentiles of thermal conductivity as a function of scale; see Sundberg et al. (2008b).

Similarly, examples of thermal property results for the objective of **prediction** are:

- Most likely thermal conductivity values at specific locations in the prediction volume, e.g. in subvolumes around deposition holes. This can be estimated for different scales.
- The statistical distribution of possible values at specific locations or subvolumes (representing the uncertainty), with corresponding statistical parameters (the mean, percentiles etc). Distributions can be created for different scales.
- The probability of encountering thermal conductivity values lower than a defined threshold at specific locations.

The main results for the objective of **visualisation** are visualisation of individual realisations of thermal conductivity, both in the model volume as a whole and at specific locations or subvolumes of interest.

5.12.3 Input to thermal numerical modelling

The modelling results includes a large number of realisations of the thermal property distribution for several deposition tunnels. These can be used directly as input to thermal numerical modelling. Such an approach keeps the entire correlation structure intact in the thermal data. This was performed in both Forsmark and Laxemar during the site selection process. The procedure is described in Section 2.5. This approach makes it possible to:

1. Verify that the temperature demands on the bentonite buffer is fulfilled by estimating the effective thermal conductivity for each canister.
2. Investigate the possibility for optimization.

An independent pre-step to thermal dimensioning can be performed in a relatively simple manner by using a developed ranking procedure, similar to that used in the thermal dimensioning of the repository; see Section 2.5. Possible outcome from the procedure contains the weighted effective thermal conductivity of each individual canister and the proportions of the rock types in different sub volumes. The methodology means that an overview of all canisters is obtained, and that the probability of different effective thermal conductivities can be estimated at canister level, as a complement to the results in Section 5.12.2 and 5.12.4.

5.12.4 Lithological properties in the model volume

For the objective of description, lithological results may include:

- Proportions of TRCs, based on simulation results (e.g. Back et al. 2007) or borehole data (Sundberg et al. 2008a).
- Uncertainty in TRC proportions, expressed as confidence intervals. This can be calculated from borehole data using the bootstrap method (Sundberg et al. 2008a).
- Typical lengths of rock bodies (TRCs) in the principal directions. This can be estimated by numerical "drilling" through randomly selected realisations of the lithology, as illustrated by e.g. Back et al. (2007).
- Distribution (histogram) of lengths of rock bodies (TRCs); see Back et al. (2007).
- Size distributions of TRCs (volumes of rock bodies). This was performed by Sundberg et al. (2008a) for subordinate rock types. The approach requires both small scale and large-scale lithological simulations in order to capture the full span of rock body sizes.

Similarly, examples of lithological results for the objective of **prediction** are:

- Most likely rock type (TRC) at a specific location in the model volume.
- Probability of encountering a specific rock type (TRC) at a specific location in the model volume.
- Probability of encountering a rock body (TRC) of a specific volume or length in a planned borehole or at a specific canister location.

For the objective of visualisation, the same applies as for thermal properties above.

5.13 Handling of anisotropy in the modelling

5.13.1 Introduction

The main types of anisotropy are described in Section 4.3.4 and in Part 2 (Chapter 6 in Back et al. 2022). The rock mass at Forsmark have anisotropic thermal properties of the following two types:

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 and is further discussed below.

The anisotropy due to orientation of rock bodies (type 2 above) is handled when the spatial statistical structure of the TRCs geology is modelled, according to Section 5.6. This type of anisotropy can also be quantified by an anisotropy factor.

However, including rock occurrence in TRCs may cause less lithologic anisotropy in the model (and thus less thermal anisotropy). This was investigated in Part 2 (Back et al. 2022). The risk of underestimating anisotropy when considering rock occurrence within the main rock type is judged to be small.

5.13.2 Anisotropy due to foliation/lineation

All rock types in domain RFM029 and RFM045 at Forsmark have been subjected to some degree of ductile deformation, both lineation and foliation. The preferred alignment of mineral grains produced by this deformation may result in anisotropy in thermal transport properties.

The directional dependence of thermal properties caused by lineation/foliation within the granite at the Forsmark site has been investigated in a large-scale field experiment, combined with laboratory and field testing at a smaller scale (Sundberg et al. 2007). A summary of the results and evaluation can be found in Back et al. (2022). A distinct scale dependence has been indicated in the investigations, which means that the anisotropy factor is significantly lower at a larger scale compared to the small scale, see Table 5-1.

Table 5-1. Results of investigation with regard to the scale dependence of thermal conductivity (Sundberg et al. 2007). Factor of anisotropy and the effective thermal conductivity (geometric mean of the two principal directions).

Scale	Thermal conductivity Mean factor of anisotropy $\lambda_{pa}/\lambda_{pe}$	Geometric mean W/(m·K)
Centimetre scale	1.40	3.45
Decimetre to metre scale	1.15	3.42

$\lambda_{pa}/\lambda_{pe}$ = thermal conductivity parallel to the foliation divided by thermal conductivity perpendicular to the foliation.

A plausible explanation for the scale dependence is that the foliation is more clearly defined at the centimetre scale compared to the larger scale. However, the variability in anisotropy still appears to be quite large at the decimetre to metre scale.

5.13.3 Handling of anisotropy due to foliation/lineation

Introducing anisotropy in the thermal modelling implies a more complex modelling; see Part 2 (Back et al. 2022). Three different data sets of thermal conductivity are required for each rock type, one for each principal direction. This puts demand on both the thermal anisotropy data for all significant rock types, the thermal modelling methodology, and the computer capacity.

Thermal data on anisotropic properties are very sparse at Forsmark. In order to consider introducing anisotropy in the thermal modelling, much more data is required.

The following requirements related to data should be met:

- Much more anisotropy data for each rock type or TRC.
- There must be significant anisotropy in the supplementary thermal conductivity data.
- The supplementary data must comprise the variation of anisotropy in different parts of the rock mass.

Until these requirements are met it is recommended that the anisotropy is handled by the end users of the thermal model in a comprehensive manner, e.g. in the thermal dimensioning. However, since data are very sparse, more data are needed even for schematic use.

5.14 Key uncertainties in the modelling

5.14.1 Data uncertainty

By data uncertainty is here referred to uncertainty in a single measurement, as well as uncertainty in a data set (multiple measurements). The objective of a single measurement is to describe the property if interest at a specific point or small volume. The data set on the other hand is a statistical sample from the target population of a specified volume of rock and should be a representative set of data describing that population. This means that data uncertainty is not only associated with the measurement technique but also with the selection of data locations in space. This applies to both thermal data and lithological data.

Data uncertainty in the thermal modelling does primarily concern:

- Thermal conductivity data – different types of data, collection principles etc.
- Thermal diffusivity data.
- Heat capacity data.
- Thermal anisotropic properties.
- Boremap data (lithological data).
- Density logging data.

Other types of thermal properties that are associated with uncertainty are the thermal expansion coefficient and temperature.

Uncertainty in single measurements is primarily a function of measurement technique. TPS measurements on isotropic samples are considered quite reliable, especially thermal conductivity. Larger errors are expected, from experience, in the TPS determination of thermal diffusivity (e.g. sensitivity to small changes in contact resistance). This has impact on the determined heat capacity that is calculated from the thermal conductivity and diffusivity from TPS measurements. However, heat capacity can also be determined directly by a calorimetric method and such measurements are expected to be more reliable. The uncertainty in thermal conductivity associated with SCA data is significantly larger than for TPS data. In addition, there is also uncertainty in the thermal anisotropic properties, mainly due to few determinations. Mean values of the thermal anisotropic factor may be quite reliable but the spatial distribution has large uncertainties. Regarding Boremap data, data uncertainties in the lithological information are generally low.

Uncertainty in the data set, i.e. the sample from the target population, is mainly a function of the number of data and how these data locations have been selected. Two principally different selection approaches exist: Probabilistic selection (random selection) and judgmental selection (subjective selection). The probabilistic approach results in a data set that is unbiased regarding the target population. Judgmental selection, on the other hand, may introduce some bias.

In Forsmark, the selection of borehole locations and borehole directions will probably be made by a mixture of random and judgmental selection approaches. This means that some data sets can be expected to be biased. Depending on how the borehole locations and directions are decided, this could be a substantial source of uncertainty, especially for lithological data. This could influence the proportions of different rock types and the size distribution of rock bodies, most importantly for subordinate rock types. This type of bias is expected to be much smaller for thermal data because the borehole locations and directions are probably decided based on lithology and given layout of the repository (the latter fine-tuned relative to defined technical design requirements), not on thermal properties of a certain rock type.

Data uncertainty in single measurements can be reduced by using a measurement technique with low systematic and random errors. Uncertainty in the data set can be reduced by collecting more data and by selecting data locations based on probabilistic principles.

5.14.2 Model uncertainty

Several of the steps in the thermal modelling are associated with model uncertainty, but its importance differs significantly between the various steps. Some uncertainties do only have a minor effect on the result, or no effect at all, whereas others are fundamental.

The presented thermal modelling methodology makes possible the study of each uncertainty quantitatively by varying both the uncertain parameters (hard data) and expert knowledge (soft data), and their effect on the output result. However, this is a slow, tedious, and labour-intensive process. Realistically, such detailed analysis could only be performed on a subset of the uncertainties and other uncertainties evaluated qualitatively.

The major model uncertainties are associated with:

1. The simulation scale (model resolution).
2. The simulation volume.
3. The definition of TRCs.
4. The assignment of TRCs to lithological data.
5. The statistical models of TRC lithology.
6. The statistical models of thermal properties.
7. The simulation technique.

Uncertainties 4 and 5 are dependent on uncertainties associated with the representativeness of boreholes and samples, as well as lack of data; see Section 5.14.1. Each of the seven model uncertainties are discussed below.

The simulation scale

Deciding a simulation scale, i.e. a size of a grid cell, in simulations introduces a discretisation error due to approximation. It is often difficult to assess how much uncertainty is introduced by approximations (Morgan and Henrion 1990). However, information theory suggests that the spatial resolution of a model must be at least twice the wavelength of the highest spatial frequency that is to be modelled (Morgan and Henrion 1990). For the thermal modelling, this implies that predictions made at the grid cell scale will be uncertain. This uncertainty is especially important regarding rock occurrences that may occur at a scale smaller than the simulation scale. Such rock occurrences will of course be underestimated due to the discretisation error. This uncertainty is reduced when several grid cells are the scope of prediction. In order to describe the size distribution of subordinate rock types in an accurate way it is necessary to perform simulations at a number of different scales.

The simulation volume

The limited simulation volume could potentially influence the simulation result. There are two situations when the limited simulation volume could be a problem:

1. When the lithological simulation volume is so small that the statistics of this limited rock volume deviate from the statistics of data. This could happen if the simulation when data from several boreholes (or tunnels) are used to derive the statistical models of TRC lithology but the simulation volume is much smaller.
2. When the correlation length (range) of thermal conductivity is similar to, or longer than, the length of the simulation volume. Experience indicates that variograms are difficult to reproduce if simulation volumes are small (Dowd P 2007, personal communication).

Both these uncertainties are reduced if the simulation volume encompasses several tunnels.

The definition of TRCs

There is an important restriction in the methodology that has implications on the definition of TRCs: Only a limited number of TRCs can be handled in the lithological simulations. This means that some TRCs has to include rock types with significantly different thermal properties. This could result in TRCs with a wide span of the thermal conductivity distribution. In Part 2 (Back et al. 2022), the result of a test is presented regarding this issue. The conclusion is that the thermal conductivity distributions may be somewhat skewed, but the statistical models can be used in the stochastic simulations without major concerns.

The assignment of TRCs to lithological data

Assigning TRCs to lithological data can be performed with different approaches; see Part 2 (Back et al. 2022). The associated model uncertainty will depend on the method used. It is expected that the method suggested in Section 5.4.5 is associated with negligible model uncertainty.

Upscaling (change of support)

Upscaling could be a major source of uncertainty, but it is difficult to assess how important it is. Therefore, upscaling should be avoided, if possible.

If upscaling cannot be avoided, great care should be taken. A check that the results are reasonable should always be made. One way could be to calculate "correction factors" (Myers 1997) from the upscaling and compare them to the upscaling performed in other subvolumes, or during the site descriptive modelling (Back et al. 2007).

The statistical models of TRC lithology

There are several uncertainties associated with the statistical modelling of TRC lithology. Most of these are coupled to the lack of knowledge concerning detailed geological information, such as typical lengths of rock bodies in the three spatial directions, representativeness of the borehole information for the modelled rock volume, and lithological heterogeneity within the rock volume. The latter is related to the variability in proportions of TRCs. In the simulation volume, the proportions of TRCs are held constant in each realisation. In reality, the proportions are variable in space due to lithological heterogeneity. These uncertainties are largest for rock types with low proportions. One way of handling lithological heterogeneity is to divide the rock volume into subvolumes, as discussed in Section 5.6.

One of the most important uncertainties for the result in Forsmark (domain 45) is associated with how the amphibolite is modelled. Analysis of typical lengths of amphibolite rock bodies could be an important aspect in the modelling. In addition, the anisotropy due to subordinate rock bodies is mainly a result of how the amphibolite is modelled. Limitations in the modelling of the spatial statistical structure of amphibolite also results in uncertainty regarding lithological anisotropy; see Section 3.2.

An approach to handle the uncertainties is to use "best estimates" of lithological parameters, determined in cooperation with geologists. Potential bias in the expert knowledge is thus transferred to the simulations of the TRC lithology. Another approach is to use alternative lithological models, representing the uncertainty in the lithology (expert opinion). For example, uncertainty in the statistical models of TRCs could be handled by performing simulations with alternative representations of transition probabilities. Each model could be weighted according to its likelihood of being correct. An alternative, or complement, is to perform a qualitative uncertainty analysis by comparing the statistics of different boreholes.

The statistical models of thermal properties

Limited data for some TRCs result in uncertain spatial statistical thermal models. When data are few and show large variability, the shape of a histogram cannot only be based on hard data. In addition, the lower limit of thermal conductivity of a TRC is usually not known and must be determined based on expert knowledge. The variograms require even more data. The assumption that thermal conductivity exhibits a similar correlation structure as density is reasonable but is associated with uncertainty.

The statistical models are influenced by approximation, which is a source of uncertainty. Important approximations are made concerning fitting of distribution models to histograms, and fitting of variogram models to experimental variograms. Such uncertainties could be reduced by collecting more data. The uncertainty could be assessed by performing simulations with alternative model functions and comparing the results.

In the case heat capacity is modelled, uncertainties associated with the thermal conductivity modelling will also affect the modelled heat capacity distribution. In addition, there are uncertainties regarding the relationship between thermal conductivity and heat capacity.

The simulation technique

All simulation methods have an effect on the output and may introduce their own artefacts (Dowd P 2007, personal communication). The uncertainty is minimised by using validated simulation algorithms and skilled personnel. The advantage of this type of uncertainty compared to the others is that it can easily be identified. The principle is simple: The result of a simulation is compared against the input models. Deviations, either random or systematic, indicate that there is uncertainty in the simulation technique. This type of verification can be performed both for the lithological and the thermal simulations.

This type of uncertainty is believed to have only a minor influence on the results, possibly larger effect for the lithological simulations than the thermal because modelling material properties (TRCs) is more challenging than modelling continuous properties (thermal conductivity).

5.15 Model evaluation and confidence-building

A model can never be validated in the sense that it is proven to represent and predict reality (Nordstrom 2012). However, the confidence in the model can be gradually increased by testing and evaluating the model. This can be done, among other things, by analysing model assumptions, by assessing the reasonableness of the results, and by comparing the results with measurements and statistics.

Evaluation of the thermal model can be performed at two levels:

1. Comparing the outputs from the individual steps in the thermal modelling procedure with data or statistics.
2. Comparing the final results of the thermal model with field measurements, i.e. a validation data set.

Outputs from the individual steps in the methodology can be analysed in different ways. For example, statistics of simulation results can be compared against the model statistics, variograms of simulation results can be checked against the variogram model, results derived by conditional simulation can be compared with a validation data set acquired from boreholes (cross-validation) etc. Examples of these methods were demonstrated by e.g. Back et al. (2007).

Evaluation of the lithological simulations (step 7; Section 5.9) can be made by performing simulations in rock volumes where the true properties are known, using conditional simulation. This is performed by removing hard data and performing simulation in order to study to what extent the removed data can be accurately predicted. The proportion of correctly predicted cells is a measure of the performance. The correctness in the predictions will increase as more and more cells are assigned true properties. In its simplest form, one borehole is used but the approach could be extended to two or more boreholes or tunnels. One way is to carry out a test for a tunnel pilot hole, with subsequent mapping of the completed tunnel. Evaluation of the lithological simulations can also be performed by analysing the statistical distribution of lengths and volumes of rock bodies in stochastic realisations (see Section 5.12), and comparing them with statistics of field observations and geological expert knowledge.

Similarly, the thermal simulations (step 8; Section 5.10) can be evaluated by comparing the simulation results with measurements of thermal conductivity, using conditional simulation. The principle is the same as above. In addition, the merged results, i.e. the output from the thermal model, can be compared to field measurements of thermal conductivity. If such measurements are of high quality, the result of the comparison will give an indication of the performance of the thermal model.

Deviations between model results and measurements should trigger evaluation of the model assumptions. If deviations are large the assumptions may be questionable, implying that the thermal model may need to be adjusted. In this way, the thermal model can be continuously improved over time.

6 Data requirements

6.1 Thermal SDM Forsmark 2007

The following data were available and used in the thermal unconditioned site descriptive simulations during the site investigations (e.g. Back et al. 2007):

- Lithological data
  - Core logging data (Boremap data) from all boreholes (rock type and rock occurrence).
- Thermal data
  - Thermal conductivity and diffusivity laboratory measurements on core samples (TPS method).
  - Calculated thermal conductivity from mineral composition (SCA method).
  - Thermal conductivity field measurements (Multi probe method).
  - Measurements of heat capacity in laboratory.
- Density data
  - Density logs from all cored boreholes.
  - Density measurements on samples.

Boremap data formed the basis for lithological simulations. Thermal conductivity data, from measurements and calculations, created property distributions for different TRCs. Such data were also utilized for analysis of the spatial correlation, as a basis for the thermal conductivity simulations.

Density logs were used to support, or replace, variogram models derived from thermal measurements since such data were sparse for some rock types. The density logs were also used to distinguish between the different sub types of TRC 51. Density measurements on samples were used to calibrate the density log and to investigate relationships between density and thermal conductivity. Heat capacity measurements were used to create a relationship with thermal conductivity, which could be used to calculate the distribution of heat capacity from the thermal conductivity realisations. Sparse data from field measurement with the multi probe method were mainly used to determine possible anisotropy in the thermal conductivity.

6.2 Data requirements for conditioned modelling

6.2.1 Aspects on thermal data requirements

The following aspects are considered particularly important and desirable:

- Sufficiently large and flexible measurement scale to enable conformity between the data scale and the simulation scale.
- Continuous thermal conductivity profiles to provide input to variogram modelling, enable subdivision between subtypes of some rock types (e.g. granite, granodiorite, tonalite, 101051) and to provide reliable distributions.
- Heat capacity measurement on samples with known thermal conductivity to provide a reliable relationship between the two, in order to calculate the distribution of heat capacity from thermal conductivity realisations

6.2.2 What data can different methods provide?

To be able to perform conditioned modelling, both thermal and lithological data are required for the specific simulation volume of interest. However, during initial stages conditioned thermal data may be sparse but lithological data from the simulation volume is a prerequisite. In Table 6-1, different aspects on thermal data are presented.

Table 6-1. Aspects on different types of thermal data described.

Type of data	Scale	Continuous profile in borehole or on core	Upscaling to simulation scale	Modelling of thermal conductivity distribution	Modelling of variogram	Determine boundaries for sub type of some TRC2
Lab data						
TPS method	cm	No	Required	Yes	No	No
Optical scanning	0.1–1 m	Yes	Probably not required	Yes	Yes	Yes
Field measurements						
DTS-Heat	0.1–1 m or larger	Yes	Not required	Yes	Yes	Yes
Density log	0.1–1 m or larger	Yes	Not required	No[1]	Yes	Yes

[1] Only possible if a reliable relationship between thermal conductivity and density logging data can be determined, in combination with density log of high quality.

From Table 6-1, the following conclusion can be made:

- Field measurement (DTS-H) has significant advantages for both distribution modelling and variogram modelling and is the preferred choice of data for conditioned modelling. However, the method needs development in order to fulfil SKBs demands (Sundberg 2019). The optical scanning method (Popov 1985) is a laboratory method that may provide similar data but has not yet been used by SKB.
- Laboratory and density log data can together provide a reasonable data base for the thermal modelling, although with some shortcomings.

6.2.3 Representativeness of data

Conditioned data

To perform a fully conditioned modelling both lithological and thermal data need to be specific to the actual simulation volume. The simulation may also be partly conditioned, especially during the initial stages of the operational phase, meaning that simulation volume specific data may be missing to some extent.

Different scenarios can be set up from different starting points. These can be divided into e.g. the following:

- Scenarios based on data access (types and scale of data, flow of data etc).
- Scenarios based on simulated rock volume. The volume may be limited in the initial stages but subsequently grow up to the annual production of pilot holes).
- Scenarios based on planned modelling intervals etc. This is further developed in Back et al. (2022), Application scenarios.

Bias in orientation – Expert judgement

In Sections 3.2 and 5.4.4 are described why lithological data can be expected to be biased; see also Chapter 4 in Part 2 (Back et al. 2022). Bias in the information used for estimating spatial statistical properties of lithological categories (TRCs) due to boreholes deviating from anisotropy directions can be corrected for in T-PROGS by transformation of the model domain to the anisotropy directions. However, there will still be bias needed to be corrected for since more information will by necessity be available from the vertical or sub-vertical directions than the horizontal directions, especially in the initial stages of repository construction. The bias is expected to decrease when the number of horizontal boreholes increases, as the construction of the repository progresses. This is valuable. However, in the specific and limited modelling volume, new borehole information will primarily represent horizontal directions during the development of deposition areas, supplemented by vertical and much shorter pilot holes in canister positions, both subparallel to the foliation. Therefore, there will be a potential bias in the total data set. This bias may increase as the number of horizontal boreholes increases.

Expert elicitation is a method that can be explored for improving the information and decreasing bias regarding spatial statistical properties such as lengths, orientations and proportions of lithological units. It is suggested that the SHELF method is considered to be used for expert elicitation.

A more exhaustive description of potential bias, as well as the SHELF method, is presented in Part 2 (Back et al. 2022).

6.3 Suggested data requirements for conditioned thermal modelling

6.3.1 Construction phase

During the construction phase, the data collection is focused on verifying the models developed during the earlier site descriptive modelling.

Data are required in order to:

- Verify the thermal site descriptive model:
  - Thermal conductivity, heat capacity and density measurements on important rock types.
  - Measurements on foliated/lineated samples of the main rock type to determine anisotropic properties.
- Verify that the pressure dependence on measurement results from water saturated samples is small, in the interval 15–100 MPa (see Section 4.3.3):
  - Thermal conductivity measurements on dry, water saturated and pressurized samples.

6.3.2 Operational phase

In addition to existing data used for earlier Thermal SDMs (see Section 6.1), the following hard and soft data are needed for conditioned modelling during the development of deposition areas (motives for data requirements are given in Section 6.2):

- Lithological data:
  - Boremap data from cores in all additional boreholes and especially boreholes in the simulation volume (rock type and rock occurrence).
  - Expert elicitation (e.g. the SHELF method).
- Thermal data:
  - Thermal conductivity field measurements in continuous profiles (DTS-Heat), in pilot holes for tunnels and deposition holes.
  - Thermal conductivity laboratory measurements in continuous profiles where field measurements are not available (Optical scanning).
  - Thermal conductivity TPS measurements on control samples.
  - Thermal conductivity anisotropy field measurements (Multi probe method).
  - Measurements of heat capacity on core samples in laboratory.
- Density data:
  - Density logs limited to boreholes where thermal conductivity measurements have not been performed for any reason.
  - Density measurements on core samples.

In Part 2 (Back et al. 2022), application scenarios, with possible data uses in the initial stages of the construction of the repository, are described.

7 Key aspects and recommendations

7.1 Methodology

All three specific objectives for the thermal modelling (description, prediction, and visualisation; see Section 1.2) are attained with application of the updated methodology for thermal modelling. Application scenarios of the methodology is discussed in Part 2 (Chapter 7 in Back et al. 2022).

Some key aspects on the methodology are:

- The statistical description of the thermal properties of a rock volume can be performed quantitatively using stochastic simulation. The result of the modelling is a large number of equally probable realisations of the thermal property distribution in the modelled volume.
- The methodology takes into account the spatial size distribution of rock type bodies and the spatial variability of thermal conductivity within each rock type.
- Prediction of thermal properties in a specific rock volume can be performed using conditioned data in the stochastic simulations.
- Measurements representing different scales can be handled using the change of support approach (upscaling), but can be avoided using continuous profiles of thermal data which provide data at the simulation scale.
- The proposed stochastic approach for thermal modelling has a high degree of transparency and flexibility. The main reasons are the stepwise approach and the combination of lithological and thermal simulations, which allows for problem-specific adjustments.
- 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.
- Expert knowledge is an important supplement to hard data in the methodology, see Section 5.5.

7.2 Recommendations for the operative phase

Some specific conclusions can be made for applying the thermal modelling methodology during the operative phase. The same basic principles for modelling can be used as during (surface-based) site descriptive modelling, but with some important differences and additions:

- The simulation scale (grid size) should preferably be 1 m, or close to that. This has major advantages. The resolution will be fairly good while keeping the simulation times at reasonable levels. In addition, thermal data may possibly be available at the same scale, which implies that there is no need for upscaling of thermal data.
- The definition of Thermal Rock Classes (TRCs) take both rock type and rock occurrence into account in a single TRC. This means that Boremap data can be used directly. This eliminates many of the uncertainties and difficult assessments in the earlier methodology and simplifies the process of defining TRCs.
- Conditional stochastic simulation should be performed, both for lithological and thermal simulations. This makes it possible to make local predictions based on conditioning data in the surrounding rock mass.
- In addition to existing data used for earlier Thermal SDMs, simulation volume specific thermal and lithological data are needed, i.e. pilot borehole data. Additional thermal data are preferably field data with the DTS-Heat method at the 1 m scale. If such data is not available, optical scanning is suggested.
- Important uncertainties in the thermal modelling are coupled to the availability of data, both the types of data and the amount of data (see Section 6.3), and the representativeness of data (bias; see Section 5.14). Bias in data is expected due to non-random location and orientation of boreholes. It is suggested that this bias is reduced by expert elicitation.

7.3 Recommendations for technical update and model validation

- The developed methodology, in the present report, needs to be tested and evaluated, e.g. for a test case in a pilot study. In this way, technical auditing of the modelling work is rendered possible. The implementation of the methodology for a test case may clarify issues of special importance and difficulty for the description and prediction of thermal transport properties.
- The DTS-Heat method needs to be further developed regarding e.g. robustness and accuracy, see Section 4.4.3 and Sundberg (2019), and the optical scanning method needs to be analysed according to SKB demands (e.g. applying coating, measurement scale).
- The result of the thermal modelling forms the basis for the thermal dimensioning (see Section2.5) and the resulting realisations can be used directly in numerical modelling. A ranking procedure was used as a pre-step to the numerical modelling during the thermal dimensioning (SKB 2009) and gave rise to a large amount of dimensioning data. Processing such information should provide an improved understanding of the possibilities for optimization of distances between tunnels and deposition holes in the repository, see Section 2.5.3. Both the numerical model and the ranking procedure needs refinement and further development.

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SKBdoc documents will be submitted upon request to document@skb.se.

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