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Thermal Site Descriptive Model

A strategy for the model development during site investigations

Version 1.0

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April 2003

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author and do not necessarily coincide with those of the client.

Abstract

Site investigations are in progress for the siting of a deep repository for spent nuclear fuel. As part of the planning work, strategies are developed for site descriptive modelling regarding different disciplines, amongst them the thermal conditions. The objective of the strategy for a thermal site descriptive model is to guide the practical implementation of evaluating site specific data during the site investigations. It is understood that further development may be needed.

The model describes the thermal properties and other thermal parameters of intact rock, fractures and fracture zones, and of the rock mass. The methodology is based on

- estimation of thermal properties of intact rock and discontinuities, using both empirical and theoretical/numerical approaches, and
- estimation of thermal processes using mathematical modelling.

The methodology will be used and evaluated for the thermal site descriptive modelling at the Äspö Hard Rock Laboratory.

Summary

SKB is performing initial site investigations in order to evaluate different sites' suitability for complete site investigations and final disposal of spent nuclear fuel. As part of the planning work, strategies are developed for site descriptive modelling with respect to different disciplines, amongst them the thermal conditions.

The objective of the presented strategy is that it should guide the practical implementation of evaluating site specific data during the site investigations. It is understood that further development may be needed.

Most of the requirements for the strategy are general to all disciplines. The strategy:

- is developed for needs connected to siting and building of a KBS-3 type repository in crystalline rock,
- should be adapted to the iterative and integrated character of the Site Investigation and Site Evaluation programme,
- should allow full transparency of data gathering, management, interpretations, analysis and the presentation of results, and
- should make use of experiences gained.

It should also be noted that the Thermal Site Descriptive Model concerns prediction of parameters. Evaluation of thermal modelling connected to Design or Safety Assessment is done elsewhere and is not part of the Site Descriptive modelling.

Components of the Thermal Site Descriptive Model

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

The thermal site descriptive model should include the temperature distribution, boundary conditions and the thermal properties of the rock mass. The boundary conditions are described by geothermal heat flow, and by temperature and climatic conditions at the ground surface. The temperature is the result of the thermal processes in the repository area. Thus the prediction should focus on variations in rock mass properties, for intact rock as well as different kinds of discontinuities, on a canister deposition scale of 1–10 m, and the boundary conditions.

The thermal site descriptive model contains the following parts:

- Geometrical framework.
- Property distribution.
- Spatial distribution.
- Description of uncertainties.

Thermal properties of the rock mass

Thermal transport properties (thermal conductivity, heat capacity, thermal diffusivity) can be determined by:

- Laboratory measurements.
- Field measurements.
- Modelling from mineralogical composition and distribution.
- Modelling from density logging.
- Modelling from temperature logging.

There are different types of laboratory methods to determine thermal properties. The method recommended for the site investigations is the TPS (transient plane source) method /SKB, 2001/.

Field measurements are performed by thermal probe methods or thermal response tests. A heat-generating probe with a temperature gauge is inserted into the ground. The thermal properties are evaluated from the relationship time versus temperature. The multi-probe method makes it possible to evaluate the thermal properties of the rock in different directions and over joints. The method of thermal response tests has been suggested as a potential thermal characterisation method. A known quantity of heat is supplied to a water-filled borehole per unit-time, and the temperature increase is measured with time. A mean value of the thermal conductivity is evaluated for the rock mass around a borehole.

Assuming isotropic and homogeneous conditions, the thermal conductivity can be calculated from the mineral composition. Based on all available measurements from Äspö HRL an empirical relationship between density and thermal conductivity and volumetric heat capacity respectively has been derived /Sundberg, 2003/. Temperature logging in boreholes is used primarily to measure the temperature distribution in the rock mass and the geothermal gradient. However, there is a clear relationship between temperature, depth, heat flow and thermal properties in the rock mass. Temperature logging can theoretically be used as an indicator of variations in thermal properties along the borehole.

Continuous improvement

The presented strategy for a thermal site descriptive model, as well as tools to improve the strategy, has to be tested and evaluated for a real case, e.g. the prototype repository at Äspö HRL.

The implementation of the strategy for a test case will clarify issues of special importance and difficulty for the predictions of thermal properties. More than one approach for predicting thermal properties of rock can be tested.

‘Technical Auditing’ (TA), i.e. examining the technical content to establish if it is adequate for the purpose, and ‘Quality Assurance’ (QA), i.e. checking that procedures are followed in line with the product realisation principle, plus the review of anomalous results, are essential tools for quality control.

It is a fundamental principle of the Site Descriptive modelling that there is consistency between different discipline descriptions (e.g. the geological, thermal, hydrogeological and hydrogeochemical descriptions). The thermal model will be partly based on the geological and hydrogeological models.

Conclusions

- The uncertainty about variations of thermal transport properties in different scales is quite large.
- Density logging seems to be a promising method to evaluate the spatial distribution, scale factors and variations in thermal properties of the rock mass. A potential method is also the evaluation of thermal property variations from temperature loggings.
- Demands on the accuracy of the estimations of thermal properties are dependent on absolute values of these properties. For high thermal conductivities of the rock mass a smaller number of data-values are probably sufficient compared to if the thermal conductivities are close to the suitable indicators in /Andersson et al, 2000/.
- The proposed strategy for thermal site descriptive model, as well as the tools to improve the strategy, has to be tested and evaluated for a real case, preferably the prototype repository at Äspö HRL.

Recommendations

- The knowledge of scale factors and spatial distribution of thermal properties need to be increased.
- Density logging seems to be a promising method to evaluate the spatial distribution, scale factors, and variations in thermal properties of the rock mass. A study mainly based on existing material is needed to analyse limitations in the proposed empirical method.
- In connection with the initial site investigation, predictions of the thermal conductivity variations should be made, based on temperature logging results.
- The thermal site descriptive model should be tested for the prototype repository at Äspö HRL. This includes a prediction of the thermal function of the prototype repository and an evaluation of the thermal properties from backward calculation.

Sammanfattning

SKB har inlett platsundersökningar för värdering av olika platsers lämplighet för fördjupade undersökningar och slutligt förvar av använt kärnbränsle. Som en del i planeringsarbetet har SKB utvecklat strategier för platsbeskrivande modellering för olika discipliner, bland dem termiska förhållanden.

Syftet med strategin är att den ska ge vägledning vid den praktiska implementeringen av utvärdering av platsspecifika data i samband med platsundersökningarna. Det kan noteras att ytterligare utveckling av strategin kan komma att behövas.

De flesta krav som kan ställas på strategin är giltiga för alla discipliner. Strategin:

- utvecklas för behov relaterade till lokalisering och byggande av ett KBS-3-förvar i kristallint berg,
- ska anpassas till de stegvisa och integrerade platsundersöknings- och platsutvärderingsprogrammen,
- ska tillåta full öppenhet avseende datainsamling, styrning, tolkning, analys och presentation av resultat,
- ska utnyttja erhållna erfarenheter.

Det bör också noteras att den termiska platsbeskrivande modellen omfattar uppskattning av värden på parametrar. Utvärdering av termisk modellering kopplad till projekteringen av förvaret eller säkerhetsanalysen görs på annat håll och är inte en del av den platsbeskrivande modelleringen.

Den platsbeskrivande termiska modellens komponenter

Temperaturen och temperaturfördelningen är central för projekteringen av slutförvaret och har också påverkan på den bergmekaniska stabiliteten, grundvattenflöden, biologisk aktivitet och kemiska reaktioner.

Den termiska platsbeskrivande modellen inkluderar temperaturfördelning, randvillkor och termiska egenskaper hos bergmassan. Randvillkoren definieras genom geotermiskt värmeflöde samt temperatur och klimatförhållanden på markytan. Temperaturen beror av termiska processer i området kring slutförvaret. Uppskattningen fokuseras på variationer i bergmassans egenskaper, både för intakt berg och olika diskontinuiteter i berget, i kapselskala 1–10 m, och på randvillkoren.

Den termiska platsbeskrivande modellen innefattar följande delar:

- Geometriskt ramverk.
- Fördelning av egenskaper.
- Fördelning i rummet.
- Beskrivning av osäkerheter.

Termiska egenskaper i bergmassan

Termiska transport egenskaper (värmekonduktivitet, värmekapacitet, värmediffusivitet) kan bestämmas genom:

- Mätning i laboratorium.
- Mätning i fält.
- Beräkningar från mineralsammansättning och mineralfördelning.
- Beräkningar från densitetsloggning.
- Beräkningar från temperaturloggning.

Det finns olika typer av laboratoriemetoder för bestämning av termiska egenskaper. För platsundersökningarna rekommenderas TPS-metoden (transient plane source) /SKB, 2001/.

Mätning i fält utförs med sondmetoder eller termiskt responstest. En värmegenererade sond med innesluten temperaturgivare installeras i marken. Värmekonduktiviteten erhålls från uppmätt temperaturökning mot tiden. Flersondsmetoden gör det möjligt att utvärdera termiska egenskaper i olika riktningar och över sprickor i berget. Termiskt responstest har föreslagits som en karakteriseringsmetod. En känd värmemängd tillförs ett vattenfyllt borrhål per tidsenhet, varmed temperaturökningen mäts som funktion av tiden. Ett slags medelvärde utvärderas för värmekonduktiviteten i bergmassan runt borrhålet.

Om man antar isotropa och homogena förhållanden kan värmekonduktiviteten beräknas från mineralsammansättningen. Ett tydligt samband mellan densitet och värmekonduktivitet respektive volymetrisk värmekapacitet har tagits fram, baserat på samtliga tillgängliga mätningar vid Äspö HRL, av /Sundberg, 2003/. Temperaturloggning i borrhål utförs primärt för att mäta temperaturfördelningen i bergmassan och den geotermiska gradienten. Det finns emellertid ett tydligt samband mellan temperatur, djup, värmeflöde och bergmassans termiska egenskaper. Temperaturloggning kan därför teoretiskt användas som en indikator på variationer i de termiska egenskaperna utmed borrhålet.

Kontinuerlig förbättring

Den presenterade strategin för en platsbeskrivande termisk modell, liksom verktyg att förbättra strategin, måste provas och utvärderas för ett verkligt fall, till exempel prototypförvaret vid Äspö HRL.

Implementeringen av strategin för ett testfall, innebär att frågor av särskild betydelse och svårighet för prognos av de termiska egenskaperna tydliggöras. Det är också möjligt att prova fler än ett angreppssätt för prognostisering av bergets termiska egenskaper.

Viktiga verktyg för kvalitetskontrollen är: ”teknisk granskning”, dvs undersökning av det tekniska innehållet för att fastställa om det är lämpligt för sitt ändamål, ”kvalitetssäkring”, dvs kontroll av att procedurerna för genomförandet följs, samt granskning av anomala resultat.

Det är en grundprincip för platsbeskrivande modellering att det finns konsistens mellan de olika beskrivningarna för de olika disciplinerna (t ex geologiska, termiska, hydrogeologiska och hydrogeokemiska). Den termiska modellen kommer till viss del att bygga på de geologiska och hydrogeologiska modellerna.

De olika disciplinernas modellbeskrivningar samt konstruktion och säkerhetsanalys är starkt relaterade till varandra.

Slutsatser

- Det finns en relativt stor osäkerhet vad gäller variationer i termiska egenskaper för olika skalor.
- Densitetsloggning bedöms som en lovande metod för att utvärdera rumsfördelning, skalfaktorer och variationer i bergmassans termiska egenskaper. Utvärdering av termiska egenskaper från temperatur loggnings resultat är också en potentiell metod.
- Krav på noggrannheten hos uppskattningen av de termiska egenskaper beror på absolutvärdet för dessa egenskaper. För höga värden på värmekonduktiviteten räcker det med ett mindre antal värden jämfört med om värmekonduktiviteten ligger nära de s k lämplighetsfaktorer som angetts av /Andersson m fl, 2000/.
- Den föreslagna strategin för en plastbeskrivande termisk modell, och verktyg för att förbättra strategin, måste provas och utvärderas för ett verkligt fall, företrädesvis prototypförvaret vid Äspö HRL.

Rekommendationer

- Kunskapen om skalfaktorer och de termiska egenskapernas fördelning i rummet behöver utvecklas.
- Densitetsloggning bedöms som en lovande metod för att utvärdera rumsfördelning, skalfaktorer och variationer i bergmassans termiska egenskaper. En studie främst baserad på tillgängligt material fordras för att analysera begränsningar hos den föreslagna empiriska metoden.
- En prognos av the termiska egenskapernas variation från temperatur data rekommenderas i samband med de inledande platsundersökningarna.
- Provning av den termiska modellen på prototypförvaret vid Äspö HRL. Detta inkluderar en prognos över prototypförvarets termiska funktion och en utvärdering av de termiska egenskaperna genom bakåtberäkning.

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1 Introduction

The Swedish Nuclear Fuel and Waste Management Co (SKB) is responsible for the handling and final disposal of the nuclear waste produced in Sweden. Site investigations have started during 2002 /SKB, 2000a/. The site investigations are carried out in different stages /SKB, 2001/ and shall provide the knowledge required to evaluate the suitability of investigated sites for a deep repository. The technique for long-term storage of spent nuclear fuel is developed at the Äspö Hard Rock Laboratory.

The interpretation of the measured data is made in terms of a site descriptive model covering geology, rock mechanics, thermal properties, hydrogeology, hydrogeo-chemistry, transport properties of the rock and surface ecosystems /SKB, 2001/. The site descriptive model is the foundation for the understanding of investigated data and a base for planning of the repository design and for studies of constructability, environmental impact and safety assessment.

This report presents a strategy for predicting the thermal aspects of the site descriptive model. The strategy for a rock mechanics site descriptive model /Andersson et al, 2002/ has been used as an example for the structure of the present report.

Parallel to this study, a thermal site descriptive model is developed for the Äspö HRL. The experiences from the development of the Äspö model are not fully implemented in the present strategy report. The strategy for the thermal model may be revised with respect to the results of the Äspö model as well as the experiences gained from the initial site investigations.

1.1 Objectives and scope

The objective of this report is to present a strategy for developing the Thermal Site Descriptive Model within the SKB Site Investigation Programme. The strategy shall guide the evaluation of site specific data.

There are several requirements for the strategy. Most of them are general to all disciplines formulating the Site Descriptive Modelling Strategy:

- The strategy is developed for needs connected to siting and building of a KBS-3 type repository in crystalline rock, with focus on the conditions to be expected at the sites selected for site investigations /SKB, 2000a/. The strategy should provide the site specific properties needed for design and safety assessment. However, this currently reported strategy focuses on the needs for thermal modelling.

- The strategy should be adapted to the iterative and integrated character of the Site Investigation and Site Evaluation programme /SKB, 2000b/. It should be able to incorporate a gradual increase in measured data, so that early predictions are revised when new data become available. Predictions should be consistent with those made in other disciplines (mainly geology and hydrogeology).

- The strategy should allow full transparency of data gathering, management, interpretations, analysis and the presentation of results. The interpreted parameters should cover the entire model domain, not just in the proximity of measuring points. Spatial variability, as well as conceptual and data uncertainty due to sparse data, errors and lack of understanding should be handled and illustrated.

- The strategy should make use of experiences gained, e.g. from the SKB Äspö project.

It should be noted that the Thermal Site Descriptive Model concerns prediction of properties. Evaluation of thermal modelling for design or safety assessment is not part of the thermal site descriptive modelling.

The objective of the strategy is to produce a thermal model that can be used for mathematical modelling of the temperature field in and around the repository with sufficient certainty. This means that the thermal properties and their estimation have to comply with requirements from design and safety assessment.

1.2 Thermal properties and processes to be predicted

1.2.1 Definitions

Thermal conductivity and heat capacity is 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 level temperature differences. It is defined as the ratio between thermal conductivity and volumetric heat capacity:

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

The geothermal gradient (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 part of the Earth. The natural geothermal heat flow in Sweden is mainly a vertical process and governed by the equation:

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

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

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

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

1.2.2 Thermal properties of rock and other parameters

The thermal site descriptive thermal model should include the temperature distribution, boundary conditions and thermal properties of the rock mass. The temperature is the result of the thermal processes in the repository area. Thus the prediction should focus on rock mass properties, including the intact rock as well as different kinds of discontinuities, and the boundary conditions. The boundary conditions are represented by the geothermal heat flow and by temperature and climatic conditions at the ground surface.

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

Table 1-1. Listing of thermal properties and parameters that should be predicted by the Thermal model, including some initial suggestions for acceptable uncertainty values. For definitions see 1.2.1.

Parameter	Unit	Scale, see 1.2.4	Suggestion for acceptable uncertainty
Thermal transport properties			
Thermal conductivity	W/(m·K)	Canister scale & repository scale	±10% if λ>3 W/(m·K) ±5% if 2.6<λ<3 W/(m·K) <±5% if λ<2.6 W/(m·K)
Heat capacity	J/(m^3·K) or J/(kg·K)	Canister scale & repository scale	±10% but better accuracy is suitable for low λ
Thermal diffusivity	m^2/s		
Thermal convection. Mass flow in water bearing fracture zones and the temperature of the water	kg/s and ºC	Tunnel scale – repository scale	±50%
Temperature			
Temperature in the rock mass	ºC	Tunnel scale	±1ºC
Temperature gradient	ºC/m	Repository scale	
Boundary conditions			
Geothermal heat flow	W/m^2	Repository scale	±10%
Temperature and climate conditions at the ground surface	ºC	Repository scale	±10%
Other thermal properties			
Internal heat production in the rock	µW/m^3	Repository scale	±20%
Thermal expansion of rock	m/(m·K)	Tunnel scale	±20%
Other relevant properties			
Density and porosity	kg/m^3 and %	Canister – repository scale	±5%

The thermal properties should be determined for different thermal elements:

- Intact rock at different scales.
- Discontinuities (fracture zones) in the rock.

Thermal data may also be necessary for the soil near the ground surface.

1.2.3 Thermal processes

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

Natural temperature field

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

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

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

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

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

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

The equation of heat conduction can be written as:

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

where
T = temperature
t = time
κ = thermal diffusivity

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

x, y, z = coordinates in space

Building the repository

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

The local temperature field in the repository depends on thermal properties of the rock and backfill, and the generated heat of the canisters due to nuclear fission. The layout of the repository is mainly dependent on the local temperature field. The design criterion is specified as the maximum temperature (100ºC) allowed on the surface of the canisters /Andersson et al, 2000/. A low thermal conductivity leads to a larger required distance between the canisters than in the case of a high thermal conductivity.

1.2.4 Relevant scales

Scale of laboratory determination of thermal properties

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

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

Preliminary the following scales are believed to be relevant:

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

Scale of thermal processes in a repository

The thermal function of a repository can be studied at different scales, exemplified in Figure 1-1. In order to describe the influence from natural climatic conditions above ground, on the thermal conditions in a repository, mean values and deviations of thermal transport properties for the whole rock mass can be representative. The sensitivity of the canister temperature for changes in the thermal properties is highest for the area close to the canister. It is therefore of special interest to analyse the variation in thermal properties in the rock mass at the scale 5–20 m (canister deposition

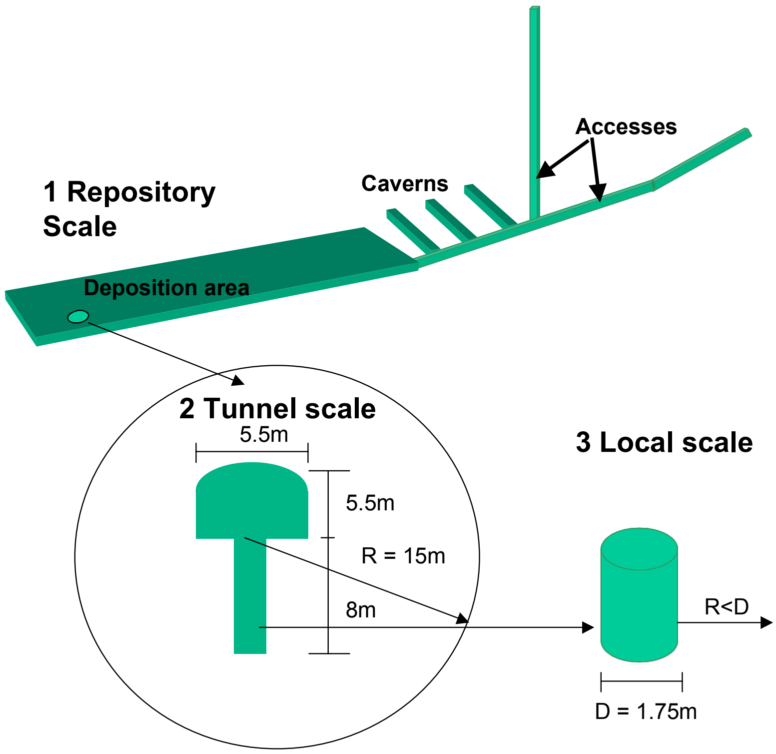

Figure 1-1. *Illustration of the various scales of importance for rock mechanics considerations for siting and constructing a KBS-3 repository /from Andersson et al, 2002/.*

scale and up to tunnel scale. Small scale variations in thermal properties is mainly averaged out in this scale.

Preliminary, the following scales are believed to be relevant:

- 1–10 m for the thermal function of the canister (canister or local scale).
- 10–100 m for the thermal function of the tunnel (tunnel scale).
- 100–1000 m for the thermal function of the whole repository (repository scale).

1.2.5 Uncertainty and required prediction ranges

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

Every parameter of Table 1-1 will be designated together with a certain degree of uncertainty. There are different kinds of uncertainties that influence the prediction of thermal properties of rock, for example:

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

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 predicted 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 prediction range of that parameter.

The required prediction range depends on the purpose of the modelling. The properties in the model need only to be predicted within the appropriate range of uncertainty. The demands on the prediction range of a property are for example lower for the modelling of natural temperature conditions than for the design distance between canisters. The demands are also dependent on the absolute level of the thermal properties. The requirements on the prediction range are higher if the level of a property is close to the suitability indicator for the siting of a repository. The suitability indicators and criteria are defined in /Andersson et al, 2000/. /Andersson, 2003/ is discussing the assessment of uncertainty in the site descriptive modelling.

If the thermal conductivity is so low that it may influence the distance between the canisters and the size of the investigation area, the demands on accuracy of the model and the property distribution are higher. In practice, this means that the investigation programme becomes more extensive.

1.3 Modelling approach

1.3.1 Model requirements

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

- Ensure that necessary properties, parameters and processes have been included.
- Allow full transparency in primary data, data flow, evaluation and presentation.
- Provide interpreted thermal data for the entire model.

1.3.2 General approach to site specific modelling

The general site investigation programme describes both investigation methods and execution programmes for the different disciplines /SKB, 2001/. Figure 1-2 shows the flow of information from site investigations to site descriptive models for various disciplines, eventually converging into a consistent site description. The information flow in the figure has been simplified. In reality, there is substantial feedback to earlier stages in the chain and exchanges of information between the different disciplines. The investigations, comprising evaluation and modelling, are executed in different stages. Design work and safety assessment analyses are carried out parallel to the information flow in the figure, and allow feedback to all stages.

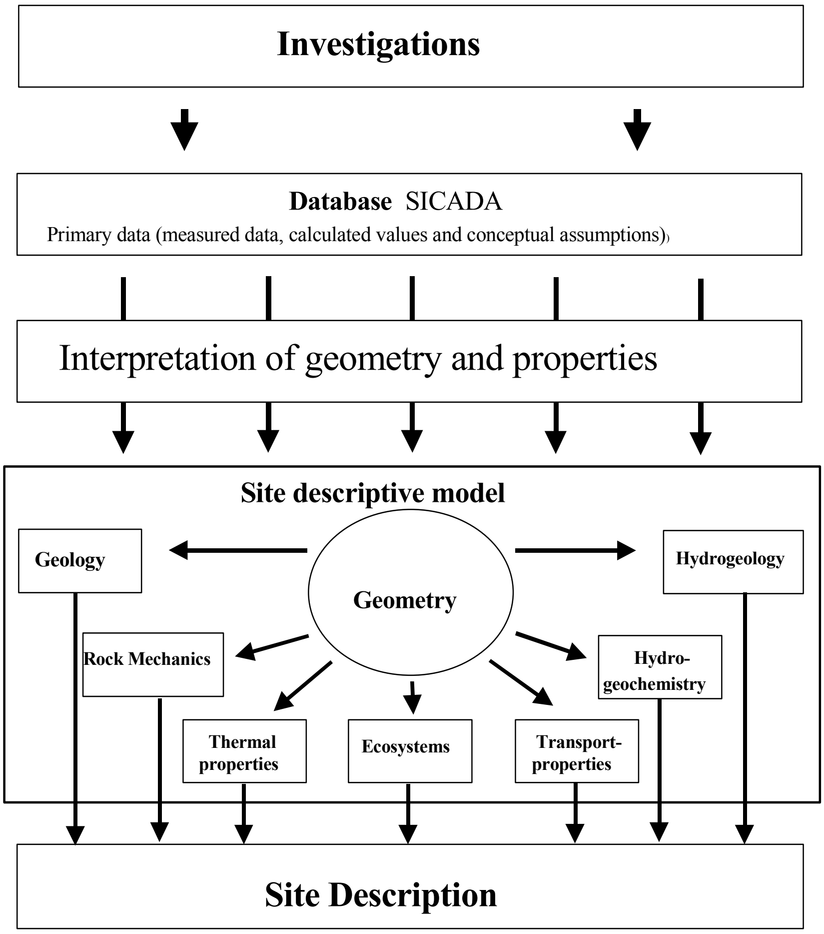

Figure 1-2. *The information flow from site investigations to site description and associated databases /SKB, 2001/.*

Figure 1-3 illustrates the activities and products during the site investigation phase. The site description is an important product of the site investigations and will be part of the documentation to be submitted together with an application for a siting permit for a deep repository.

A methodology to construct, visualise and present Site Descriptive Models has been presented by /Munier and Hermansson, 2001/. The methodology has four major components:

- Construction of a geometrical model of the interpreted main rock components (fracture zones and rock volumes between fracture zones).
- Description of geoscientific characteristics of the rock components.
- Description of the geometric uncertainties in the interpreted model structure.
- Quality system for handling the geometrical model and the associated databases.

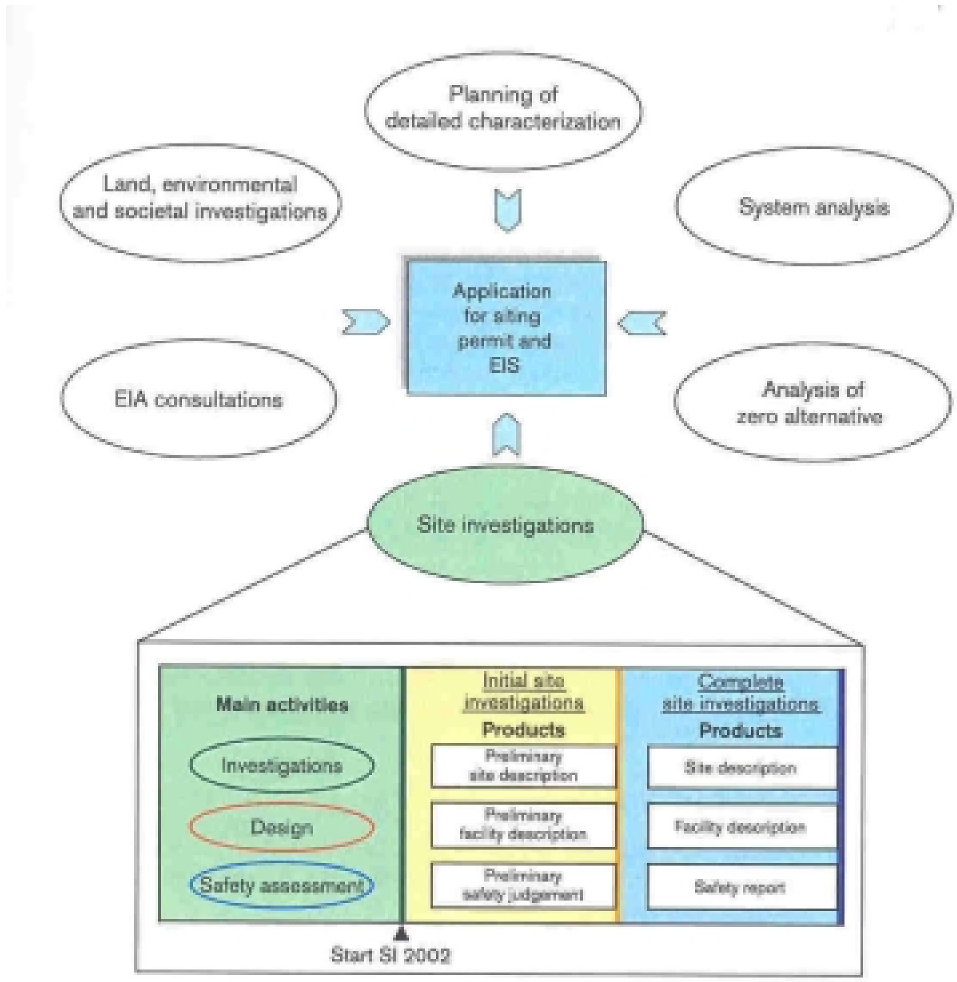

Figure 1-3. *Illustration of activities and products during the site investigation phase (SI). Activities are shown as ovals while products are shown as rectangles. EIS = environmental impact statement /SKB, 2001/.*

The site descriptive model should deal with conceptual uncertainty, data uncertainty, spatial variability of parameters and confidence in a model. The confidence in a site descriptive model is the total composition of indications and arguments in support of the model. If the uncertainty in the description of properties is high but well founded, the confidence in the model can still be high.

In /SKB, 2001/ summaries of site descriptive models for different disciplines are presented. The summary of the thermal site descriptive model is given in Table 1-2.

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

Purpose of model

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

Process description

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

Constituents of the model

Geometric framework

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

Parameters

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

Data representation

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

Boundary conditions

Initial temperature conditions and heat flow.

Numerical tools

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

Calculation results

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

1.3.3 Development of site specific thermal model

The development of the thermal model is carried out step-wise and the different model versions can be divided into the following main categories:

- Model version 0 – based on feasibility study (FS).
- Model version 1 – based on initial site investigations (ISI).
- Model version 2 – based on complete site investigation (CSI).

During the initial site investigations the thermal model is based on estimations and calculations from the geological and geophysical rock characterisation etc. The evaluation may be complemented with some direct measurement of thermal properties.

The characterisation is deepened during the complete site investigation. The site is characterised so well that the model can be used to forecast the future temperature distribution as a basis for the preliminary facility description.

2 Strategy for estimating thermal properties

2.1 Identification of input data and interaction with other disciplines

2.1.1 Overview of required data and interaction with other disciplines

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

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

The site descriptive model consists of models produced in a number of disciplines (see Figure 1-2). These models are developed jointly and iteratively, whereas refined versions are produced, during the different stages of the site investigation. The geological model and in minor extent the hydrogeological model contain valuable information for the development of the thermal model. Especially the geometrical framework and rock type description/distribution is of interest. Thermal properties and parameters are summarized in Table 1-1.

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

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

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

2.1.2 Geological and geometrical description

The geological modelling is briefly described in /SKB, 2001/ and further outlined by /Munier et al, 2003/. The geological model includes the geological evaluation and is essential to the understanding of a site. The model also includes the geometry of regional and local major fracture zones as well as the spatial distribution of rock types.

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

In the geological model, fracture zones are subdivided dependent on the size. The model only describes fracture zones larger than 1 km. Fracture zones smaller than these regional zones and local major fracture zones are only described statistically for each rock unit. The statistical description of the fractures typically comprises:

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

The statistical fracture parameters may be used to evaluate the thermal properties (mainly thermal conductivity) for non-intact rock.

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

2.1.3 Hydrogeological description

The hydrogeological description contains information on the permeability distribution in the rock mass. In the model, hydraulic properties of the different rock units in the geological model are characterised. Information is given on mass flow in water bearing zones. This information may be essential for the thermal model when the non-intact rock should be described from a thermal point of view. A hydraulic structure in the rock mass causes convective heat transport.

2.1.4 Rock mechanic description

The elevated temperature in a repository influences the stress distribution due to thermal expansion of the rock. The strategy for a rock mechanics site descriptive model is outlined in /Andersson et al, 2002/. /Probert and Claesson, 1997b/ have made calculations of thermoelastic stress for the KBS-3 repository.

2.1.5 Geophysical properties

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

Rock characterisation of individual cores is essential for the interpretation of the borehole loggings of temperature, density and porosity. Density and porosity loggings may be used to describe the spatial distribution of thermal properties in the rock mass (see 2.3.5). Rock characterisation is also used for describing the samples selected for laboratory measurements of thermal properties.

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

2.1.6 Thermal properties

Thermal properties are measured in the laboratory using core samples from intact rock. It can also be of interest to measure thermal properties of surface rock samples. It is also possible to make field measurements.

2.1.7 Surface conditions

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

2.1.8 International experiences

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

2.2 Influence on thermal transport properties

The totally dominating thermal transport process in crystalline rock is thermal conduction. Forced convection or convection by gravitation may occur in hydraulic structures.

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

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

2.2.1 Mineral content

Variations in the mineral distribution for a rock type results in differences in the thermal conductivity. Quartz has 3–4 times higher thermal conductivity than most other minerals. Thus, the quartz content normally has a great influence on the total thermal conductivity. However, at 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 Chapter 2.3.4.

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

2.2.2 Temperature

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

However, two separate studies at the Äspö HRL show no significant trend for the thermal conductivity with respect to temperature for different rock types /Sundberg and Gabrielsson, 1999; Sundberg, 2002/. The exception is altered Äspö diorite, where there is a trend towards decreasing thermal conductivity values with the temperature. The thermal conductivity increased by about 7% in the interval 25–80ºC.

Temperature dependence in the heat capacity has been found for granitic rocks at the Äspö HRL. In one study, the measured volumetric heat capacity in the laboratory increased in average 17% in the interval 25–80°C (0.31%/K) /Sundberg, 2002/. In another study on the same rock types the thermal conductivity increased by 17% in the interval 0–75°C (0.23%/K) /Sundberg and Gabrielsson, 1999/.

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

2.2.3 Porosity and pressure

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

2.2.4 Anisotropy and heterogeneity

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

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

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

The harmonic and arithmetic mean equations may be used to obtain upper and lower bounds, respectively, of the thermal conductivity of anisotropic rock.

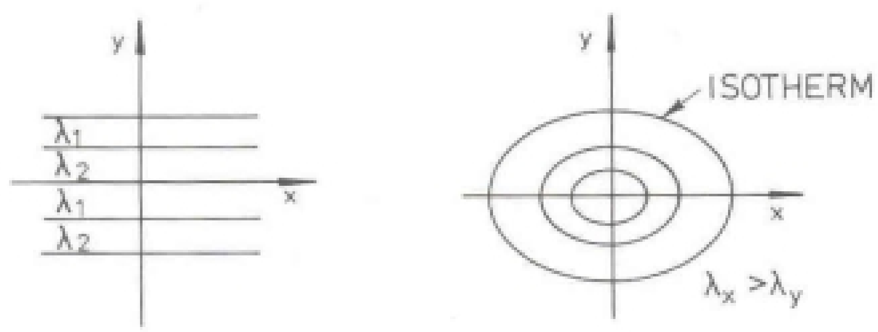

Figure 2-1. *Anisotropy /Sundberg, 1988/.*

2.3 Determination of thermal transport properties

2.3.1 Introduction

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

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

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

2.3.2 Laboratory measurements

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

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

2.3.3 Field measurements

The principle *in-situ* methods for measuring thermal properties are thermal probe methods and thermal response tests.

The *in-situ* methods usually give a characteristic value for a larger volume compared with laboratory measurements. The field methods can be used as a complement to the laboratory measurements.

Thermal probe method

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

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

The thermal properties of a fracture zone may be measured by the multi-probe method. Measurements can with this method be performed in different directions in anisotropic rocks.

Thermal response test

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

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

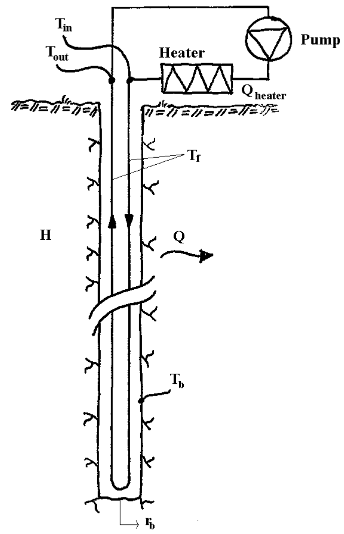

Figure 2-2. *The principle of the thermal response test /Gehlin, 1998/.*

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

2.3.4 Mineralogical composition

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

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

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

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 self-consistent approximation is in good agreement with measured values /Sundberg, 1988/. However, later investigations at Äspö HRL /Sundberg and Gabrielsson, 1999; Sundberg, 2002/ indicate a tendency for the self-consistent approximation to underestimate the thermal conductivity with about 5–8% for the actual rock types.

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

2.3.5 Density logging

Density measurements have been used as an indicator to distinguish between Ävrö granite and Äspö diorite at Äspö HRL /Rhén et al, 1997/. A relationship between density and thermal conductivity for all investigated rock types was later observed by /Sundberg, 2002/. Based on all available measurements from Äspö HRL empirical relationships between density and thermal conductivity and volumetric heat capacity, respectively, were derived in /Sundberg, 2003/ and are shown in Figure 2-3.

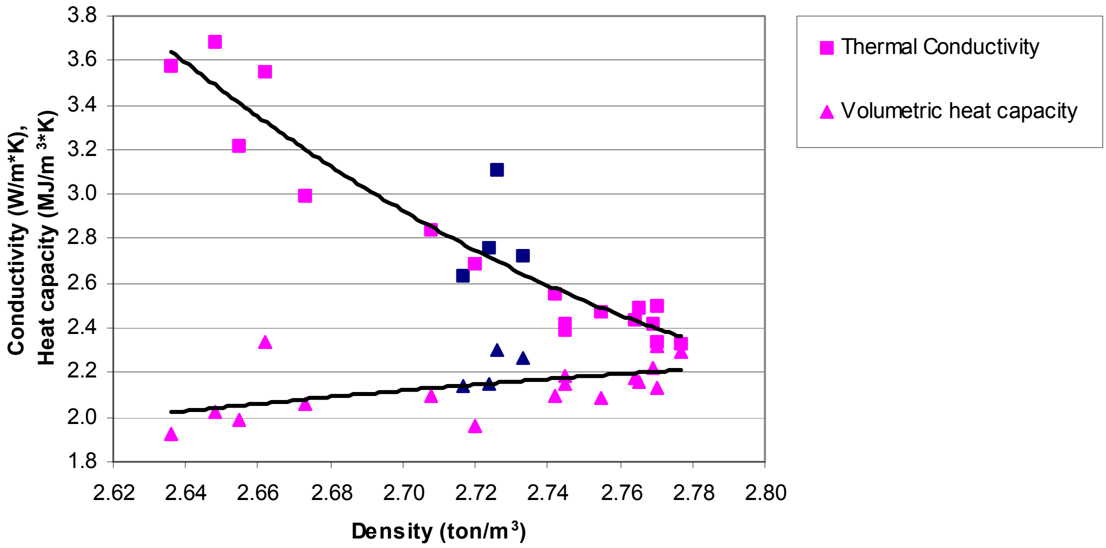

Figure 2-3. *Estimated relationships between density and thermal properties of investigated rock types at Äspö HRL. Values of altered Äspö diorite are marked with blue colour. Equations are derived by polynomial regression using all values /Sundberg, 2003/.*

The relationships can be described with the following equations:

Thermal conductivity (W/(m·K)), all values

$$\lambda = 27.265\rho^2 - 156.67\rho + 227.18 \qquad R^2=0.88 \qquad (2\text{-}3)$$

Volumetric heat capacity (MJ/(m³·K)), all values

$$C = -2.5496\rho^2 + 15.156\rho - 20.215 \qquad R^2=0.26 \qquad (2\text{-}4)$$

where ρ (ton/m³) is the density and R^2 indicates the correlation.

Using the equation (2-3) and (2-4) it is possible to calculate the thermal properties from density loggings in boreholes. An example of thermal conductivity versus depth modelled from density logging in a borehole at Äspö HRL is shown in Figure 2-4.

However, the equations are only valid for the range of densities (approximately 2.65–2.77 ton/m³) that were used to derive the equations, and for the actual rock types at Äspö HRL (Äspö diorite, Ävrö granite and Fine-grained granite). Thus the equations are not valid for rock with lower or higher density.

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

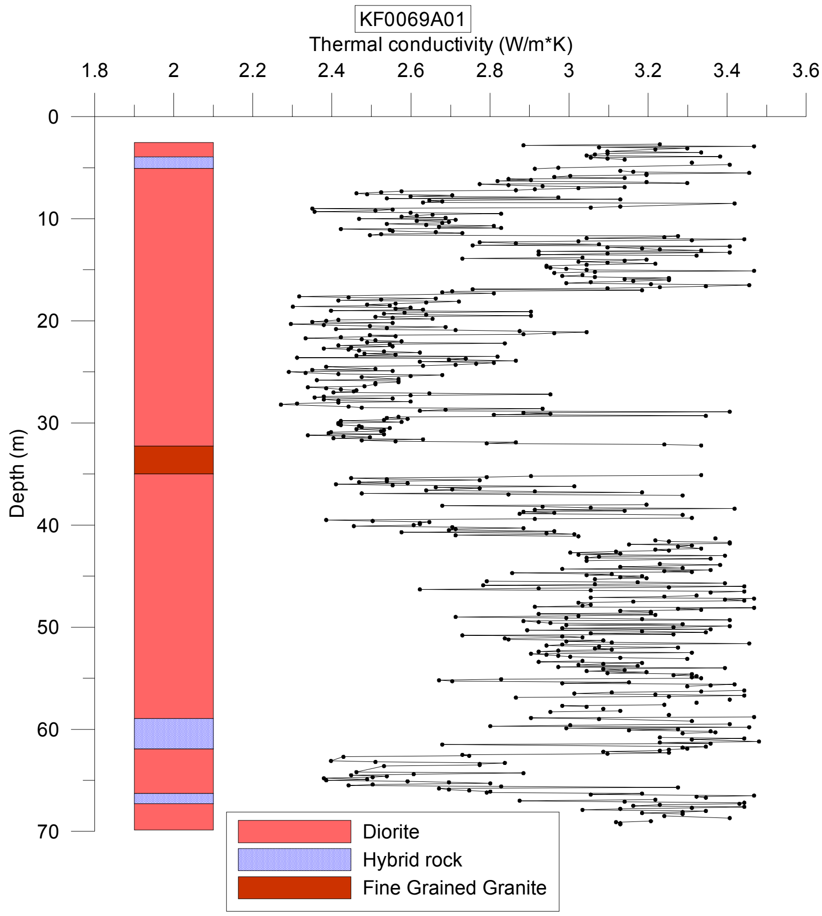

Figure 2-4. *Calculated thermal conductivity (from density logging result) versus depth for borehole KF0069A01 at Äspö HRL.*

2.3.6 Temperature logging

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

2.3.7 Correlation to rock type

Thermal transport properties can be correlated to rock type through the mineral composition (see also 2.3.4). /Sundberg, 1988/ made calculations of thermal conductivity from mineralogical composition for about 4000 samples. Tolerance intervals were created related to rock type. Thus, from the geological description of an area a ruff estimation of the thermal conductivity can be made.

2.3.8 Thermal properties of fracture zones

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

The thermal properties of fracture zones are mainly evaluated from geological and hydro geological description and from geophysical data. Theories of calculation of thermal properties of high porosity geological material is involved. The thermal properties of a fracture zone can be calculated by the geometric mean equation.

However, fracture zones will not be present near the deposited canisters. The thermal influence on the local temperature field will therefore be quite small.

2.4 Determination of temperature distribution and other thermal data

2.4.1 Temperature logging

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

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

2.4.2 Internal heat production

The internal heat production in rock can be calculated from the content and radioactive decay of Uranium, Thorium and Potassium.

Normally the internal heat production is small and has only a limited effect on the temperature distribution. However, for e.g. young granites the internal heat production may be larger.

2.4.3 Thermal expansion of rock

The thermal linear expansion is measured on core samples in the laboratory. The planned tests and measurement methods are outlined in SKB site investigation programme /SKB, 2001/. Measurements made at Äspö HRL showed no significant variation due to rock type /Sundberg and Ländell, 2002/.

2.5 Determination of boundary conditions

2.5.1 Geothermal heat flow

With knowledge of the geothermal gradient and the thermal conductivity of the rock mass it is possible to calculate the geothermal heat flow (see definitions in 1.2.1). 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 particular geology.

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

2.5.2 Climate conditions at the surface

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

2.6 Uncertainties

The uncertainties can be divided into the different groups (sections) mentioned above (see also section 4.5):

Laboratory measurement

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

Field measurements

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

Modelling from mineral content

- The accuracy in the modal analyse due to e.g. large grains, alterations of minerals.
- The chemical composition of some minerals, e.g. plagioclase has uncertainties.
- Errors in the methods and limitations of background theories.
- Insufficiencies in thermal data on minerals, especially of the heat capacity.

Density loggings

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

Temperature loggings

- Insufficiencies in the temperature calibration.
- Uncertainties in the temperature determination due to water perturbations in the borehole.

Fracture zones

- Insufficiencies in the geological and hydrogeological desriptions.
- Errors in the methods and limitations of background theories.
- Insufficiencies in geophysical data.

Thermal expansion of rock

- Performance of the tests and applied test procedures.

Geothermal heat flow

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

Climate conditions at the surface

- Predictions of future climate conditions.

3 Modelling of thermal processes

3.1 Introduction

A methodology for thermal modelling is developed with respect to the model requirements. The thermal modelling will require specific thermal data, in such an extent that the requirements of a thermal model are met. A detailed description of input parameters to the model is given in Chapter 2. Available data and interpretations from other disciplines will also be used in the thermal modelling. For example

- Structural geology model.
- Lithological model.
- Hydrogeological model.

The mathematical modelling of temperatures in and around a repository will be made in different time and geometrical scales. The "global" solution contains the large-scale temperature field covering the repository and the surroundings, and includes both short and long-term influence of boundary conditions. The local solution contains the temperature distribution on and around a canister.

The mathematical modelling can be made for the following phases:

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

The first point implies a prediction of the natural thermal conditions. However, the natural large scale thermal process is rather insensitive to errors in the determination of the thermal transport properties, the spatial distribution and the boundary conditions. In combination with expected disturbances on the temperature logging results may not be a fully reliable test on the model accuracy.

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

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

3.2 Scales

3.2.1 Representative elementary volume

For the determination of the effective thermal conductivity, it is of interest to know whether the volume used for determination is representative for the whole rock mass or not. This is achived if the representative elementary volume (REV) is estimated. REV is defined as the elementary volume whose properties are unchanged when the volume is slightly increased. The REV of rock must contain sufficient grains to yield a mean value with some statistical certainty. For isotropic normal-grained rocks, a volume of a few cm^3 would be enough. However, if the rock is heterogeneous, the REV must include a much larger volume. Thus, the REV can be quite different depending on the scale of investigations, see Figure 3-1.

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

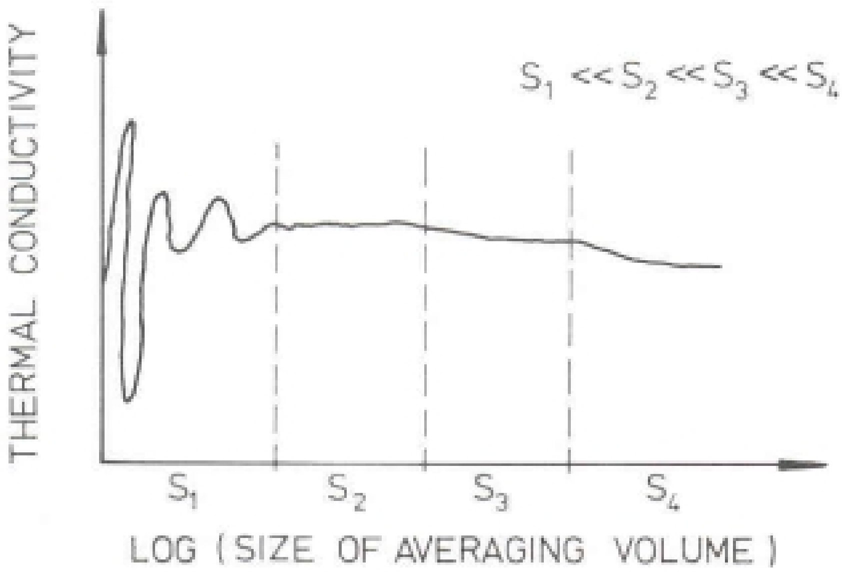

Figure 3-1. *The thermal conductivity versus average volume /Sundberg, 1988/.*

3.2.2 The large-scale temperature field – repository scale

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

3.2.3 The local temperature field – canister scale

The local temperature field is of primary concern for the design of a repository. The design criterion is specified as the maximum temperature allowed on the surface of the canisters. A low thermal conductivity leads to a significantly larger distance between canisters than in the case of a high thermal conductivity, and can in some cases also influence the size of the investigation area.

The sensitivity in canister temperature to changes in the thermal properties is highest for the area closest to the canister. It is therefore of special interest to analyse the thermal impact on the canister if there is a variation in the thermal properties in the rock mass at the canister deposition scale, 1–10 m, or if the variability occurs at a larger scale. In the first case the temperature effect of the variation in thermal properties is levelled to a rather high degree. In the second case the effect of the variations is not averaged out.

/Ageskog and Jansson, 1999/ carried out heat propagation studies for a repository in three different rock types. /Probert and Claesson, 1997/ made temperature field modelling due to time dependent heat sources for the KBS-3 repository.

In /Sundberg, 2003/, 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 m is averaged out and have small influence on the canister hole temperature. Larger blocks at a scale of 5–10 m with different thermal conductivity have a significant influence on the canister hole temperature.

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

The simulation result shows that the temperature of the canister hole is highly influenced by the thermal properties in a $6 \cdot 40\ m^2$ area around the canister. The influence is stronger closer to the canister.

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

4 Site descriptive modelling – assigning thermal properties to the rock mass

4.1 Introduction

The first step is to analyse the distribution of thermal properties for different rock types or rock domains. The next step is to distribute the properties in the 3-dimensional rock mass. The assigned thermal properties are afflicted with different kinds of uncertainties that need to be identified and assessed.

The procedures described in this chapter assume that the required property data is available. Thermal properties of rock have been determined as well as possible influences on the properties, e.g. the temperature dependence.

The thermal site descriptive model contains the following parts:

- Geometrical framework.
- Property distribution.
- Spatial distribution.
- Description of uncertainties.

4.2 Geometrical framework

The base for the geometric framework consists of the lithological and geological-structural models. The geological model is described geometrically by using a concept of rock units and rock domains. A rock unit is a volume judged to have a reasonably statistically homogeneous distribution of lithology and fracturing statistics. Fracture zones are special cases of rock units. See also Chapter 2.1.2.

4.3 Estimating the property distribution

The distribution of measured or calculated intact rock properties is analysed geostatistically and confidence intervals are created. Experiences from Äspö HRL indicate that the thermal property distribution within rock domains or rock types may not be normally or log-normally distributed /Sundberg, 2003/. In that case, a distribution-free method is needed for the analysis. However, a distribution-free method requires a larger number of observations to create a confidence interval than the case with normally or log normally distributed data.

Fracture zones may have significantly different thermal properties compared to the intact rock. However, fracture zones are not going to occur near the deposited canisters. The thermal influence on the local temperature field is therefore assumed to be small.

4.4 Estimating the spatial distribution

Three different approaches to estimate the spatial distribution of thermal properties are discussed. The spatial distribution can be estimated using:

- Geological model.
- Overall estimation of rock types for a rock domain.
- Geostatistical theory.

The geological model can be used to describe the spatial distribution of thermal properties. The geological description is divided into fracture zones and rock domains. The rock domains may be subdivided into rock types, with different thermal properties. However, a quite high degree of uncertainty may exist in the spatial distribution of rock types and this uncertainty is transferred into the thermal model. Therefore, the level of detail for the rock type description, on which the analysis should be based, is open to discussion. From a thermal point of view, the rock type definition does not have to be more precise and detailed than what is needed for the determination of the spatial distribution of thermal properties.

A another way may be to look on the whole rock domain as a unit and make a number of assumptions of the amount of different rock types and their associated thermal properties. This different approach is used to create a distribution of thermal properties within the rock domain.

An alternative method is to extrapolate point values to a rock volume using geostatistical theory and search for the correlation structure. The distribution of thermal conductivities along a borehole, for example the data in Figure 2-4 can be used to create a variogram. Variograms express the variance versus the lag (the distance between samples). Each point in the variogram represents the variance in thermal conductivity for a certain distance (lag) between the samples.

Figure 4-1 shows the variogram for thermal conductivities along the borehole in Figure 2-4, estimated from the empirical relationship with density. This example of variogram shows data points within correlation distance from one other for small and large lag lengths. In between, around a lag length of 10 m, the variance is almost constant. The "nugget" is the sum of small-scale variations (cm-dm) and measurements errors. The variogram can also be used for kriging interpolation between point values if a variogram model is fitted to the experimental variogram.

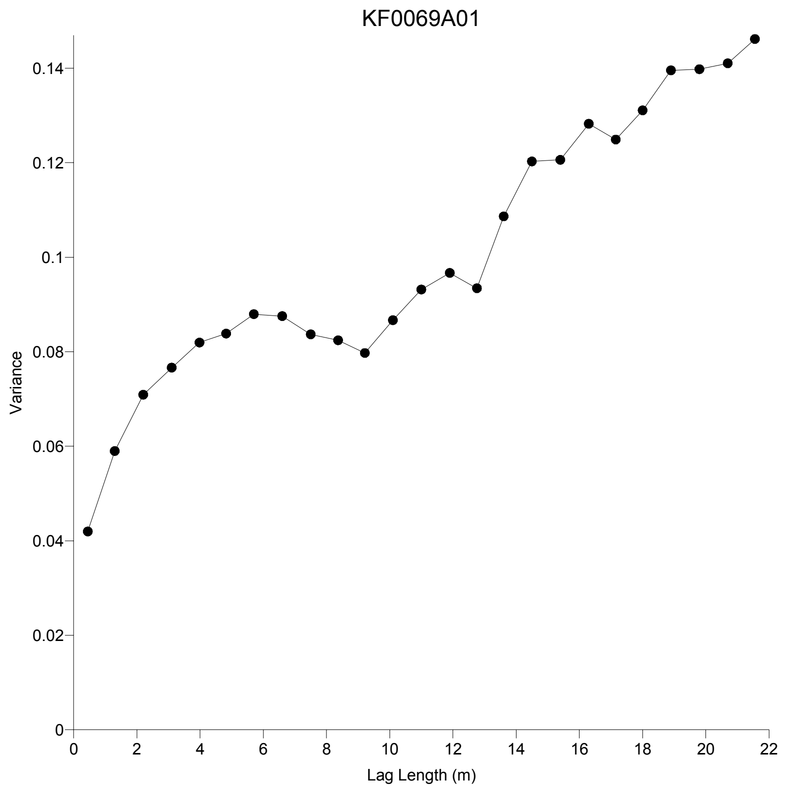

Figure 4-1. *Example of a variogram for thermal conductivities along a borehole (KF0069A01 at Äspö HRL).*

4.5 Uncertainties

There are different kinds of uncertainties when assigning values and distributions to different elements in the model. The following main uncertainties can be identified:

- Uncertainties in the conceptual model (the understanding of the place and the involved processes).
- Uncertainties in the mathematical model (the ability to describe the conceptual model mathematically).
- Uncertainties in measurement or calculation methods, both at natural temperature and at elevated temperatures (data uncertainty).
- Uncertainties in the thermal property distribution and confidence interval within rock types or rock domains.
- Uncertainties in the spatial distribution of rock types or thermal properties.
- Uncertainties of small-scale variations in thermal properties for "homogeneous" rock type and in the up scaling to a larger volume.

These uncertainties need to be identified, quantified, assessed, and handled throughout the modelling process. The data uncertainty is a source of information for the design and safety assessment and the interaction give the needs of accuracy in the thermal model. This is further described in /Andersson, 2003/.

5 Documentation and visualisation

5.1 Thermal model

A methodology to construct, visualise and present geoscientific descriptive models has been presented by /Munier and Hermansson, 2001/. The methodology has four main components:

1. Construction of a geometrical model of the interpreted main rock components (fracture zones and different volumes between fracture zones) at the Site.
2. Description of the geoscientific characteristics of the rock components.
3. Description and geometrical representation of the geometric uncertainties in the model.
4. Quality system for the handling of the geometrical model and the associated database.

The modelling work starts out from the primary data measured at the site. Fundamental for quality assurance is that data for modelling are taken from the SKB Site Characterisation Database (SICADA). Firstly, only quality-controlled data may be stored in SICADA, Figure 5-1. Archived information is maintained in accordance with quality assured procedures. Secondly, only data from SICADA may be used for interpretation, analysis and modelling of the investigated sites. The data from SICADA specifically used for the thermal model are of different types:

1. Results of laboratory testing, intact rock or samples from fracture zones.
2. Results of *in-situ* temperature measurements.
3. Results from density loggings.

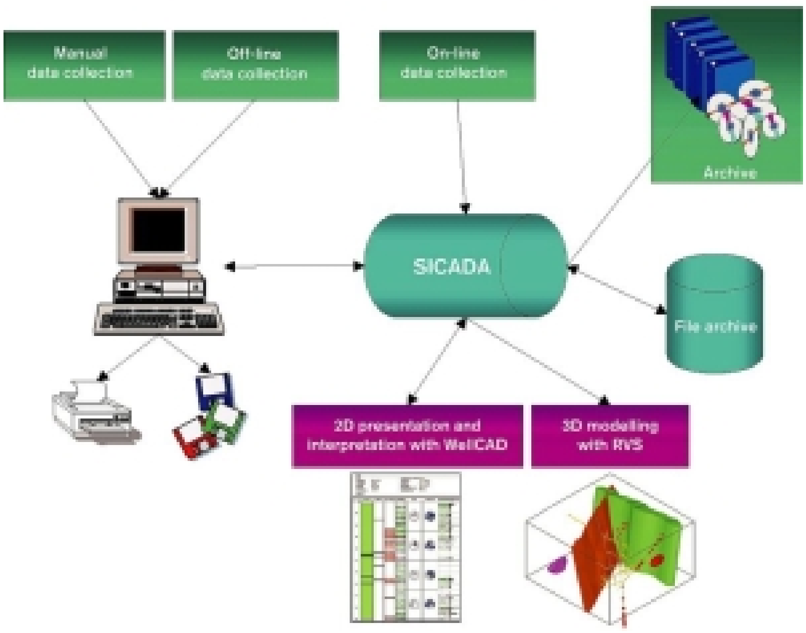

Figure 5-1. *SKB's database SICADA with associated functions /SKB, 2001/.*

A model is considered a collection of interpreted geometries. Each geometry within the model is defined by its co-ordinates. In addition, each object or geometry (i.e. deformation zone, rock unit, etc) contains a set of parameters that defines it. Values of the parameters are then given together with information on the activities that generated those specific values.

The SKB CAD based tool for visualisation, Rock Visualisation System (RVS), is used for creation and maintenance of 3-dimensional geometries, such as deformation zones, lithological boundaries, ground surface and tunnels, and interpreted data connected to these geometries (that are not stored elsewhere). RVS facilitates modelling and administration of geological interpretations and data.

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

- Input data and supporting models.
- Evaluation of primary input data and input obtained from other disciplines (geology and hydrogeology) of the Site Descriptive Model.
- Reference to the generated files and their ID in the model database.
- The documentation trail.
- A summary description of the modelling results and major uncertainties. The description of uncertainty is an integrated part of the Site Description.
- Recommendations for the next investigation step, if required.

5.2 Quality assurance

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

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

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

6 Continuous improvement of the strategy

6.1 Test case

The presented strategy for a thermal site descriptive model, as well as tools to improve the strategy, has to be tested and evaluated for a real case, preferably the prototype repository at Äspö HRL. A set of protocols describing what to model, how to model it and how to assess the quality of the results can guide the test. This way technical auditing of the modelling work is allowed. A test case was also used in the development of a rock mechanics site descriptive model, with positive results /Andersson et al, 2002/. Technical auditing and attached protocols were estimated to be potentially powerful tools.

The implementation of the strategy for a test case will clarify issues of special importance and difficulty for the predictions of thermal properties. More than one approach for predicting thermal properties of rock can be tested. It will also be possible to improve procedures for handling uncertainties. For example, higher uncertainty may be accepted for rock types that are not supposed to be in close neighbourhood to the canisters.

The work should follow the quality control procedures outlined in Chapter 5.2.

6.2 Quality control of the improvement strategy

Quality Control applied to the improvement procedures has to account for the details of both the overall Thermal Site Descriptive Model and the specific components of the Model.

A brief summary of components in a Quality Control strategy is outlined in /Andersson et al, 2002/. The strategy should contain:

- A Project Plan, Schedule and Activity Plan for the continuous improvement of the Model are necessary in line with SKB procedures. This helps to ensure that the work is well planned, understood, and directly geared to the purpose, process description and constituents of the anticipated Model at the different time periods.
- There should also be a well-established method for regularly scanning the world information on factors related to thermal properties of rock, repository site investigations, etc. Some of the information will come through SKB international meetings and personal contacts.
- The use of Protocols and/or activity plans is necessary to ensure that the implementation of the work is well structured.
- The handling of uncertainties is one of the most important issues and requires specific attention. Issues of special importance and difficulty should also be given emphasis.

- The results of ongoing modelling work should be screened on a regular basis, focussing on the need for further development. This includes team meetings, internal reviewing, periodic workshops, and external reviewing.
- Finally, there should be periodic memoranda presenting the updating approach to the Thermal Site Descriptive Model.

In the updating approach it is necessary to consider what is generic information and what is site-specific information. Generically useful information and conclusions from similar projects worldwide can be included in the approach.

6.3 Interaction with other models

It is a fundamental principle of the Site Descriptive modelling that there is consistency between different discipline descriptions (e.g. the geological, thermal, hydrogeological and hydrogeochemical descriptions). The thermal model will be largely based on the geological and hydrogeological models. The thermal modelling also provides important input to the rock mechanics and hydrogeological modelling, e.g. thermal stresses and influence on water transport. This means that each version of the Site Descriptive Model will have to build on interaction and integration of the results of different discipline teams.

The geological information comprises distribution of different rocks and how representative obtained values of thermal properties are. However, the geological information may contain uncertainties that are transferred into the thermal description. These uncertainties must be handled and taken into account. Interaction with geologists ensures good understanding of the geological site model. Thermal assumptions must be compatible with the geological representation and the hydrogeological description of the rock mass.

Detailed geological description of test sections is valuable for evaluation of the reliability of measurement results. Detailed description of drill cores (mineralogy, grain size, foliation) is necessary for the evaluation of laboratory measurements of thermal properties. The thermal modeller needs to be engaged in the overall co-ordination of core samples selected for the different tests.

7 Conclusions and recommendations

7.1 Conclusions

- There exist quite large uncertainties in the variation of thermal transport properties in different scales.
- Density logging seems to be a promising method to evaluate the spatial distribution, scale factors and variations in thermal properties of the rock mass. However today the method is restricted to certain local rock types at Äspö HRL and to a limited density range.
- Temperature logging results may under favourable conditions be a valuable method to evaluate variations in thermal conductivity.
- Demands on the accuracy of the estimations of thermal properties are dependent on absolute values of these properties. For high thermal conductivities a smaller number of values are sufficient compared to if the thermal conductivities is close to the suitable indicators in /Andersson et al, 2000/ to achieve a low deviation and an acceptable variation in the predicted temperatures.
- The proposed strategy for thermal site descriptive model, as well as the tools to improve the strategy, has to be tested and evaluated for a real case, preferably the prototype repository at Äspö HRL. After possible adjustments/supplements it is possible to present a useful strategy that can guide the practical evaluation of thermal data to a thermal site descriptive model.

7.2 Recommendations

- The knowledge of scale factors and spatial distribution of thermal properties need to be increased.
- Density logging seems to be a promising method to evaluate the spatial distribution, scale factors and variations in thermal properties of the rock mass. A study based mainly on existing material is needed in order to analyse limitations in the proposed empirical method, to study scale changes in thermal conductivity, and to extend the method to high porosity parts of the rock mass.
- It is suggested that a prediction of the thermal conductivity variation from temperature logging result is made in connection with the initial site investigations.
- It is suggested that tests are performed of the thermal model on the prototype repository at Äspö HRL. This includes a prediction of the thermal function of the prototype repository and an evaluation of the thermal properties from backward calculations.

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