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Hydrogeological Site Descriptive Model – a strategy for its development during Site Investigations

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Key words: Hydrogeology, hydrology, site descriptive model, hydraulic tests, site investigation.

Abstract

The report is to present a strategy for the development of the Site Descriptive Hydrogeological Model within the SKB Site Investigation Programme. The report, and similar reports from the Geology, Rock Mechanics, Thermal properties, Hydrogeochemistry, Transport Properties and Surface Ecosystem disciplines are intended to guide SKB Site Descriptive Modelling but also to provide the authorities with an overview of how the modelling should be performed. Thus the objectives of this report are to:

- provide guidelines for the modelling of different sites resulting in consistent handling of modelling issues during the Site Investigations,
- provide a structure for the modelling sequence that is suitable for the establishment of a Site Descriptive model and
- provide some necessary details that should be considered in a Site Descriptive model.

Sammanfattning

Rapporten redovisar en strategi för framtagandet av en Platsbeskrivande Hydrogeologisk modell inom SKB:s Platsundersökningsprogram. Rapporten, och liknade rapporter från ämnesområdena Geologi, Bergmekanik, Termiska egenskaper, Hydrogeokemi, Transportegenskaper och Ytnära ekosystem skall guida SKB:s platsbeskrivande modellering men också ge myndigheter en översikt av hur modelleringen är tänkt att genomföras. Syftet med rapporten är att:

- ge riktlinjer för modelleringen av de olika platserna så att modelleringsfrågor behandlas på ett likvärdigt sätt under platsundersökningarna,
- ge en struktur på den modelleringssekvens som är lämplig för att ta fram en Platsbeskrivande modell, och
- presentera ett antal viktiga beståndsdelar som ingår i en Platsbeskrivande modell.

Contents

1 Introduction

This report presents the general strategy for the development or design of a Hydrogeological Site Description during Site Investigations.

The Site Investigations in the Forsmark and Simpevarp areas commenced during the year 2002, and a basic site description in addition to available data has been presented /Forsmark version 0, 2002; Simpevarp version 0, 2002/. The general investigation and evaluation programme was presented in /SKB, 2000/ while the general site programme for Site Investigations was described in more detail in /SKB, 2001b/. A general overview of the site selection process and Site Investigation programme is presented in /SKB, 2001a/.

This chapter presents objectives, a brief overview of the Site Descriptions and the report structure.

1.1 Objectives and scope

The objective of this report is to present a strategy for the development of the Site Descriptive Hydrogeological Model within the SKB Site Investigation Programme. An overview of Site Descriptive Modelling and integrated evaluation strategy is reported in /Andersson, 2003/. The strategy as presented in this report should guide the practical implementation of evaluating site-specific data during Site Investigations, although it is understood that further development may be needed.

There are several requirements for the strategy. Most of them are general to all disciplines.

- The strategy should be adapted to the iterative and integrated character of the Site Investigation and Site Evaluation programme /SKB, 2000/. It should be able to incorporate a gradual increase in measured data, so that early predictions can be revised as new data become available. Predictions made within different disciplines should be consistent in an interdisciplinary context.

- The interpreted parameters should be extrapolated to cover the entire model domain, not just in the proximity of measuring points. Spatial variability, as well as conceptual and data uncertainty due to sparsly distributed data, errors and lack of understanding should be handled and visualised.

- The strategy should enhance interaction with Safety Assessment (SA), Investigations and Rock Engineering, by providing the information needed at different stages, as well as being able to handle feedback from these activities. In particular, the strategy should indicate the completion of the Site Evaluation, based on surface investigations, so that the Sites are comparable, thus forming the basis for a decision on the most appropriate site for a deep repository.

- The strategy should promote transparency of data gathering, management, interpretation, analysis and presentation of results.

- The strategy should make use of both previous experience and experience gained during the Site Investigations. It needs to be adaptable to future needs and experiences and for this reason should not be overly detailed.

It should be noted that the Hydrogeological Site Descriptive Model concerns prediction of structure geometry and parameters. Evaluation connected to Design or Safety Assessments is not part of Site Descriptive modelling. It should also be noted that the modelling strategy and this report will be updated when necessary.

This report, and similar reports from the Geology, Rock Mechanics, Thermal properties, Hydrogeochemistry, Transport Properties and Surface Ecosystem disciplines are intended to guide SKB Site Descriptive Modelling but also to provide the authorities with an overview of how the modelling should be performed. Thus the objectives of this report are to:

- provide guidelines for the modelling of different sites resulting in consistent handling of modelling issues during the Site Investigations,
- provide a structure for the modelling sequence that is suitable for the establishment of a Site Descriptive model and
- provide some necessary details that should be considered in a Site Descriptive model.

1.2 General Work Procedure

Site Investigations should provide a "Preliminary Site Description" at the end of the Initial Site Investigation and a "Site Description" after completion of the Site Investigation /SKB, 2001b/, thus forming the basis for analysis and assessments to be made by the activities Design and Safety Assessment. Table 1-1 illustrates the models. The Geology, Rock Mechanics, Thermal properties, Hydrogeology, Hydrogeochemistry, Transport Properties and Surface Ecosystem disciplines are all represented in Site Investigations, see Figure 1-1.

Parts of Site Descriptive Modelling are performed individually by the various disciplines but much of the modelling is based on close cooperation and integration between them. This report gives an overview of the interaction and integration between Hydrogeology and the other disciplines. The overall performance of Site Descriptive Hydrogeological Modelling and its interaction with other disciplines is shown in Figure 1-2.

A number of hydrological and hydrogeological methods are used to collect information for the Hydrogeological site descriptive model but it must be stressed that the evaluation of data and content is strongly linked to the Geological Site Descriptive model. The working process shown in Figure 1-2 indicates 6 main parts:

1. Primary data for hydrogeological analysis (Geoscientific Site Description (GSD)).
2. Hydrogeological analysis of primary data (GSD).
3. Integrated evaluation and Site description (GSD).
4. Data delivery (GSD).
5. Design and Safety Assessment.
6. Central Site Evaluation.

Table 1-1. Different versions of the Site Descriptive Model produced during the Site Investigation.

Phase	Basis	Covers	Product/model
Prior to Site Investigation	Feasibility studies. Processing of existing data. Field checks.	Part of municipality and candidate area for site.	General model on regional scale (Version 0).
Initial Site Investigation	General aerial, surface and short borehole surveys.	Candidate area and site (regional and local scale).	Choice of priority site within candidate area. General model (Version 1.1).
	Surface and some deep borehole investigations.	Site (regional environments).	Preliminary model on local and regional scale (Version 1.2).
			Preliminary Site Description.
Complete Site Investigation	Investigations in many deep boreholes and supplementary ground surveys.	Site. Regional environments.	Model on regional and local scale (Version 2.1).
	More deep borehole and supplementary ground surveys.	Site. Regional environments.	Revised model on regional and local scale (Version 2.2).
	More supplementary surveys.	Site. Regional environments.	Finished model on regional and local scale (Version 2.X).
			Site Description.

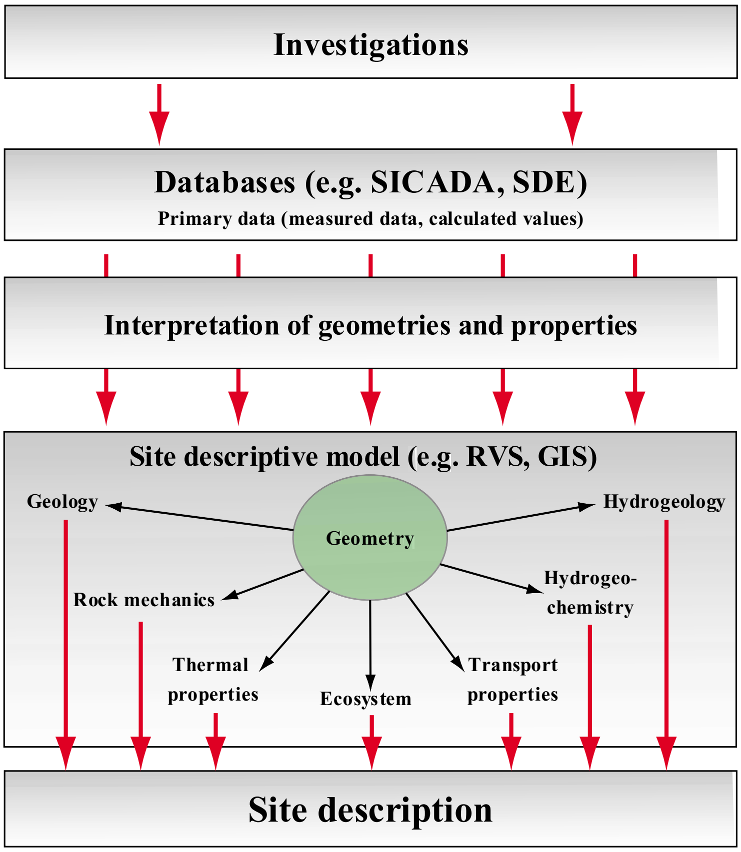


Figure 1-1. *The primary data from the investigations are collected in a database. Data are interpreted and presented in a site-descriptive model, which consists of a description of the geometry and different properties of the site.*

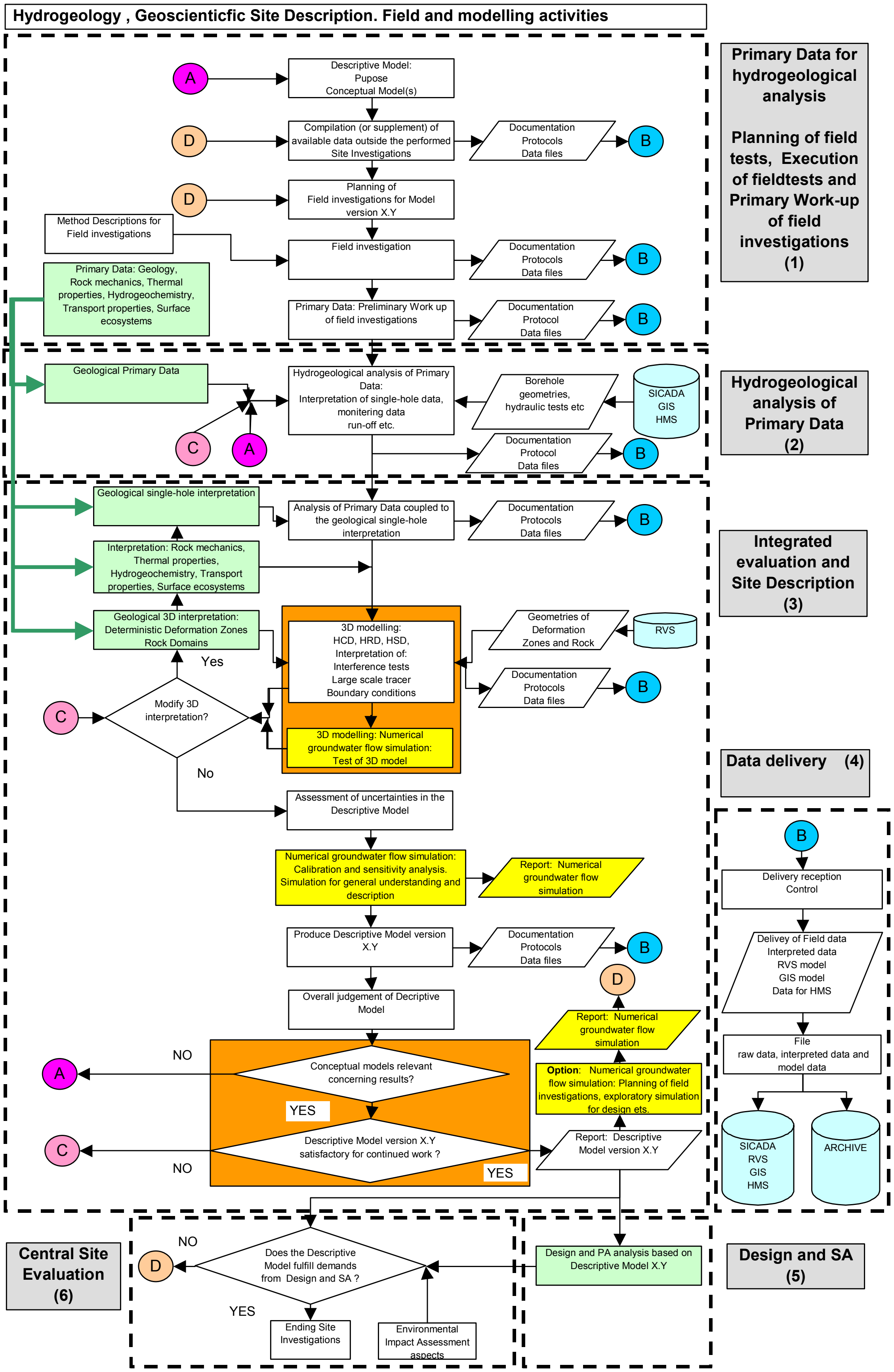


***Figure 1-2.** An overview of the general performance of Site Descriptive Hydrogeological Modelling and the interaction with other disciplines. A, B, C and D show connections in the flow chart.*

Nos 1–4 in Figure 1-2 cover the Hydrogeological part of the Geoscientific Site Description (GSD) and are described in Chapters 4–6 of this report. Nos 5–6 represent the interaction between Hydrogeological aspects and Design, Safety Assessment (SA) and Central Site Evaluation. In more detail:

No 1 covers the fieldwork and the first interpretation of the measured data leading to *Primary Data* in accordance with the Method Descriptions.

No 2 covers the analysis of *Primary Data* performed on single-hole tests, monitoring data etc that requires no interaction with other disciplines. Some geological mapping of boreholes is used in the analysis.

No 3 includes three steps:

- The first step is the interaction with geology for the interpretation of the data from the boreholes, mapping, logging and single-hole tests.
- The second step is the use of the initial geological information in the structural model in order to analyse the data in terms of 3D representation of major deformation zones and the rock between the zones. The 3D representation of hydraulic properties is tested with numerical groundwater flow simulations. The structural model will be updated as required, based on input from all disciplines, after which it may be necessary to go back to step 1 to modify the interpretation.
- The third step represents the assessment of concepts used, the groundwater flow simulations in order to increase understanding of the situation at the site, the assessment of the uncertainties as well as presenting version X.Y of the Site Descriptive Model as a report and a digital database. This step is performed when the disciplines have put forward a model that they judge to be consistent with available data and knowledge. If necessary, the numerical groundwater flow model is used for exploratory simulations to obtain useful information for new field investigations and/or to answer specific questions from the Design and SA groups.

No 4 represents data delivery from the field investigations as well as to and from the different analysis steps.

No 5 represents the work of the Design and Safety Assessment (SA), which is independent of the Geoscientific Site Investigation group. This work is based on the latest Geoscientific Site Description Model.

No 6 represents SKB's overall evaluation (Central Site Evaluation) of the results from GSD, Design and SA. A decision is made as to whether new investigations are needed or the existing descriptions and collected data are sufficient for the next step of the siting process where for example an Environmental Assessment Report is to be made on the Deep Repository.

Each investigation phase involves these 6 parts. Part 3 involves much interaction with other disciplines with successively updating of the models to achieve consistent models based on the available data.

The Site Descriptive Modelling strategy for the disciplines will be described in a number of reports similar to this report /Löfgren and Lindborg, 2003; Smellie et al, 2003; Munier et al, 2003; Andersson et al, 2002b; Berglund et al, 2003; Sundberg, 2003/.

1.3 Site Description methodology

SKB has long experience of performing field investigations and producing Site descriptions of different kinds. One early project was the International Stripa Project /Gnirk, 1993/. The siting and construction of the Äspö Hard Rock Laboratory is similar to what can be expected for the future Deep Repository /Almén et al, 1994; Stanfors et al, 1997a; Rhén et al, 1997a; Stanfors et al, 1997b; Rhén et al, 1997b; Rhén et al, 1997c/. The Site Descriptive modelling was further developed and tested in the Laxemar project /Andersson et al, 2002a/. SKB has gained experience from large scale groundwater modelling during work within the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes which is useful for the development of numerical modelling strategies /Rhén and Smellie, 2003; Gustafson and Ström, 1995; Gustafson et al, 1997/. SKB has also conducted several other large-scale groundwater modelling projects /e.g. SKB, 1999/ and presented results and experiences at international workshops /e.g. OECD, 1999/. Based on these experiences, the general site descriptive modelling strategy is outlined in /Andersson, 2003/.

Parameters that are important to consider during Site Investigations are described by /Andersson et al, 1997, 1998/. The conceptual model structure applied in the Äspö project is shown in /Olsson et al, 1994/.

An overview of the Quality Assurance (QA) of the Site Investigations is presented in /SKB, 2000/. The QA involves doing the appropriate work and also performing that work correctly. Programmes and operating plans ensure that the appropriate work is carried out, while Activity Plans (AP) ensure that the work is performed correctly.

An Activity Plan defines how an activity should be performed. It usually refers to a Method Description (MD) that, in turn, specifies SKB's general requirements in respect of the method of investigation concerned, the required degree of accuracy, the actual method of working in addition to data acquisition and processing aspects.

The geological model is essential for hydrogeology. /Munier et al, 2003/ describe geometric modelling methodology, including geological modelling definitions and RVS (Rock Visualisation System) modelling. Geometric uncertainties and the quality system for managing different versions of geometric models are also included in the report. A definition and description of geological, geophysical and rock mechanic mapping of rock parameters are provided by /Stråhle, 2001/.

Groundwater flow simulations are needed for understanding of the site as well as a part of the Site Description. Several numerical simulation codes can be used for groundwater flow modelling. Continuum codes that may be used are DarcyTools /Svensson, 2002a,b/, NAMMU /Cliffe et al, 1999/. The Discrete Fracture Network (DFN) approach will be used and the FracMan and MAFIC /Dershowitz et al, 1995/ codes may be used. CONNECTFLOW (Including NAPSAC) makes use of the (NAMMU) continuum code and a DFN code /CONNECTFLOW, 2002/.

1.3.1 Site Description input data

For each candidate area, Site Description input data comprise a compilation of data from the Feasibility Study and a re-interpretation of some existing data, thus forming the basis for the 0 version Site descriptive model /Forsmark version 0, 2002; Simpevarp version 0, 2002/ for each candidate area. Model version 0 provides a basis for the planning of the initial investigations at a specific site.

The Site Investigations will provide "Primary data" in accordance with Figure 1-2. These data are the major input for Site Descriptive modelling. Different types of investigations provide the data, while the Method Description aims guide the investigations and to be a part of the QA. The hydrogeological methods that are planned for the Site Investigation are briefly presented in Appendix 1, Table A1-1. Some methods described within the geological and transport disciplines are also mentioned in Table A1-1, as they are essential to the hydrogeological interpretation. The Method Descriptions are intended as documents for the management of Site Investigations and do not always contain detailed descriptions on how the methods are to be performed but instead include references to other documents containing details of performance and equipment.

Primary data are stored in different databases such as SICADA (Site Characterisation Database), SDE (Spatial Data Engine, the GIS database) and HMS (Hydro Monitoring System). QC of the data takes place before storage of data but the data analysis carried out in relation to the Site Descriptive Modelling is in practice another form of QC.

Chapter 4 gives an overview of the collection of Primary data.

1.3.2 Site Descriptive modelling and Site Description output data

Site Descriptive modelling is a stepwise procedure illustrated in Figure 1-2 and briefly discussed in Section 1.2. Part of the initial analysis of the Primary data can be performed by each discipline on an individual basis, but the major part of the modelling is an integrated (between the disciplines) and iterative procedure. Chapter 5 gives an overview of the initial Primary data analysis carried out by the hydrogeological discipline, and Chapter 6 outlines the integrated modelling.

A primary task for hydrogeology is to define hydraulic properties, boundary and initial conditions based on Primary Data. Equally important is the groundwater flow modelling. As soon as the first version of the site's geometric elements, hydraulic properties, boundary and initial conditions is available, this preliminary description of the site can be tested hydraulically. The *Model testing* consists of simulations of different major geometric alternatives or boundary conditions in order to try to disprove a given geometric interpretation or boundary condition. The result from this testing is useful for the internal discussion of the interpreted geometries and boundary conditions. The interaction between the Geology and Hydrogeology disciplines, but also the disciplines of Hydrogeochemistry, Transport and Surface Ecosystem, in interpreting the available data, is essential in order to obtain consistent models. When all the disciplines agree that the geometric model(s) are consistent with the available data, the groundwater flow model can be *calibrated* and a *sensitivity analysis* made. This (or these) calibrated groundwater flow model(s) can produce flow paths and flow conditions useful for the Hydrogeochemical, Transport and Surface Ecosystem Site Descriptions.

The X.Y version Site Description, with its groundwater flow models then forms the basis for further analysis by Design and SA and for the planning of new investigations. Exploratory groundwater flow simulations should be considered when planning field investigations or solving specific Design and SA questions.

The Site Description in the form of reports, the X.Y version model data base and the results from the groundwater flow modelling can be considered as "output data" for the entire Site Investigation.

1.3.3 Management of uncertainties

The parameters in the Site Descriptive model will always contain uncertainties. The uncertainties are associated with measurement and data, spatial and temporal variability and conceptual uncertainty. The management of uncertainties is described in Sections 6.5 and 6.6. A general description of the evaluation of uncertainties and /reliability is given by /Andersson, 2003/.

1.4 Report structure

Some essential terminology is presented in Chapter 2. The main concepts and parameters are discussed in Chapter 3. Chapter 4 describes the Primary data collected by means of field investigations and monitoring. The initial hydrogeological analysis of primary data is outlined in Chapter 5 and the integrated interpretation procedure is presented in Chapter 6. In Chapters 7 and 8 information and documentation management as well as the updating of this report are briefly presented.

2 Terminology

Within a multidisciplinary project, a uniform and clear nomenclature is essential to avoid misunderstanding and to promote comprehension of the studied site. This chapter summarises the meaning of some general terms commonly used within SKB in connection with the present Site Investigations and the methodology presented in this report.

2.1 Modelling scales

The Site Description covers both a *Regional Site Description* and *Local Site Description*. The Local Site Model domain description usually covers some 10 km^2 and should be detailed enough for the design of a deep repository and performance of the required SA. The Regional Site Model domain covers a large area surrounding the Local Site Model domain and is less detailed than the Local Site Description but sufficiently detailed to provide an overall view of the geological, hydraulic and other conditions in the area. The Regional Site Description provides data for the Regional Groundwater flow models that are essential for defining/testing boundary conditions for the Local Site Groundwater flow models.

2.2 Modelling domains

An essential part of the Site Description is to define the properties of the soil and rock within the Regional Site Descriptive and the Local Site Descriptive models. The division of the rock and soil (regolith) into domains is based on the fact that the difference in properties is relevant to the design of the Deep repository and/or the Safety assessment. The nomenclature that will be used for the Site Descriptive models is outlined below.

A geometric model consists of several volumes. The smallest volume within the 3D model is called a unit, see Figure 2-1. Basic Geological units may form different domains in accordance with the interpretations made by the different disciplines, see Figures 2-2 and 2-3. In /Munier et al, 2003/ the main geological definitions are outlined, some of which are included below, in addition to some hydrogeological definitions.

Deformation zone (Swedish: Deformationszon): Essentially a 2D feature with a limited thickness that has undergone a brittle and/or plastic deformation.

Rock unit (Swedish: Bergenhet): Part of the rock volume with similar properties, for example a certain rock type.

Soil unit (Swedish: Jordenhet): Part of the surficial deposits on the bedrock with similar properties, for example a sandy layer, also often referred to as Quaternary deposits in the Geological Site description. Terrestrial as well as marine and lacustrine deposits are included in the term “Soil”. (In this report, soil is treated in the geological engineering sense, i.e. as synonymous with “regolith”, which is defined as follows /Jackson, 1997/: “A general term for the layer or mantle of fragmental and unconsolidated rock material, whether residual or transported and of highly varied character, that nearly everywhere forms the surface of the land and overlies or covers the bedrock. It includes rock debris of all kinds, volcanic ash, glacial drift, alluvium, loess and eolian deposits, vegetal accumulations, and soil.” (Soil is generally equal to *Solum (Swedish: jordmån)*).

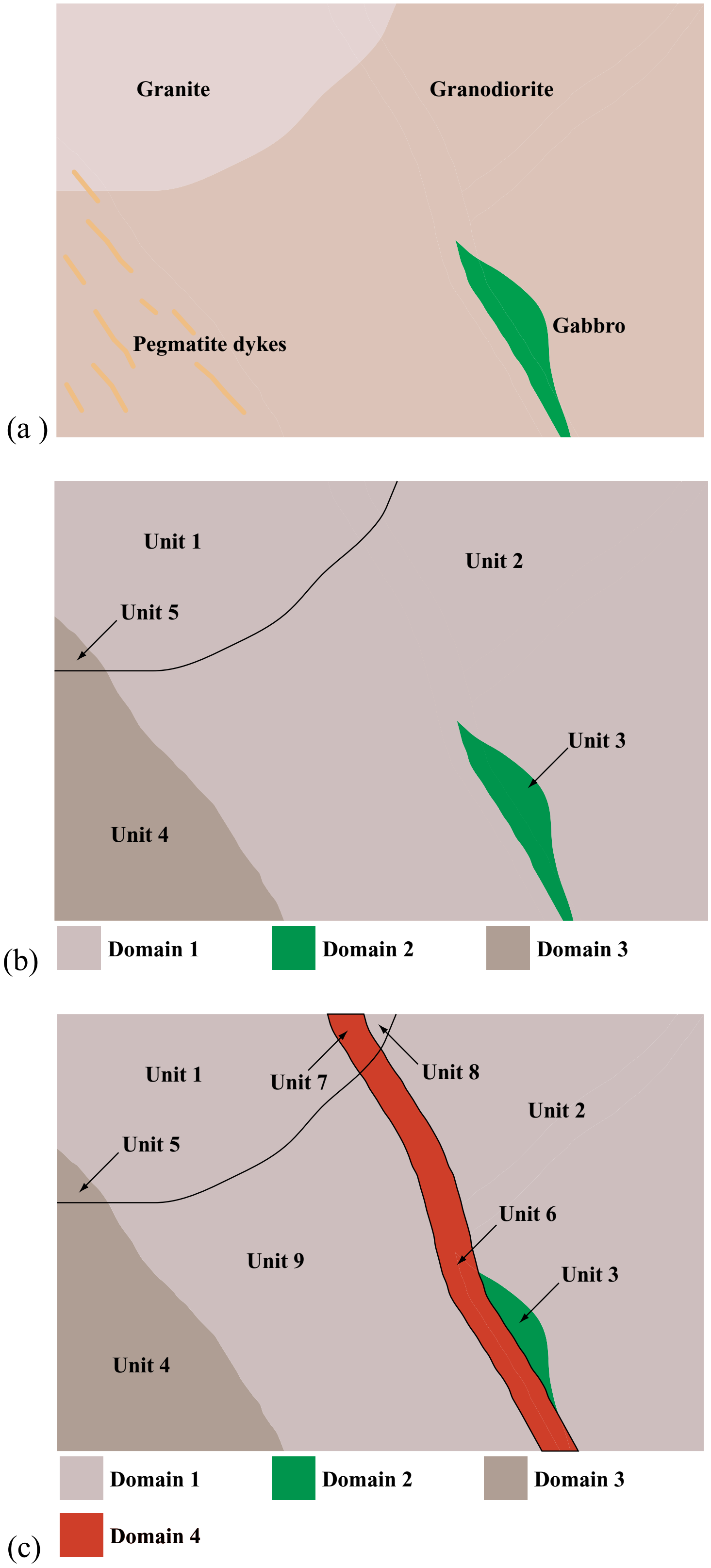


Figure 2-1. *Illustration of the concepts of units and domains. (a): A hypothetical geological map showing the distribution of a number of rock types and an area characterisiesed by swarms of granitic veins. (b): The same map subdivided into a number of rock units and 3 domains based on the physical properties and heterogenity of the bedrock. (c): The bedrock in "a" is intersected by a deformation zone, creating 5 additional rock units. /Munier et al, 2003/.*

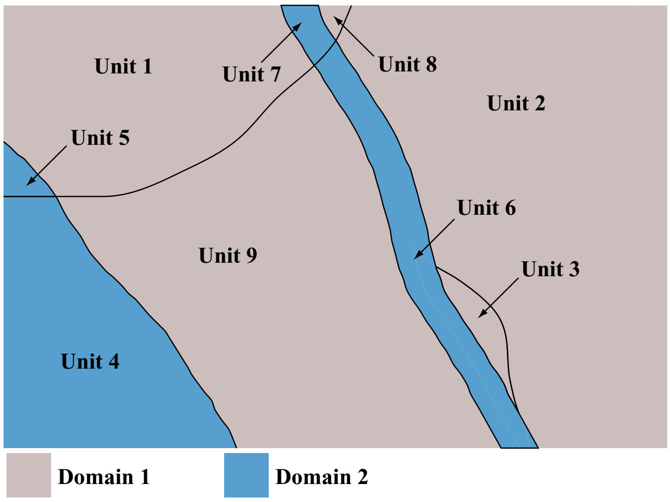


Figure 2-2. *The domains in Figure 2-2 can be described as two Hydraulic Rock Domains and one Hydraulic Conductor Domain (unit 6+8) /Munier et al, 2003/.*

Domain (Swedish: Domän): Units with similar properties may be grouped together into domains.

Hydraulic Conductor Domain (HCD) (Swedish: Hydraulisk Strukturdomän): A Deterministic deformation zone or part of a Deterministic Deformation zone with constant or defined variability of hydrogeological properties.

Hydraulic Rock Domain (HRD) (Swedish: Hydraulisk Bergdomän): A grouping of Rock Units, which are not part of the HCDs, with similar hydrogeological properties.

Hydraulic Soil Domain (HSD) (Swedish: Hydraulisk Jorddomän): A grouping of Soil Units with similar hydrogeological properties.

2.3 Hydrogeological modelling

Although the nomenclature in hydrogeology and groundwater flow modelling is fairly well established, it is not always concordant. In this section the Nomenclature used for hydrogeological modelling is outlined. Basic hydrogeological references are /Kruseman and de Ridder, 1990; Horne, 1995; Lohman et al, 1972; Wilson and Moore, 1998; ASTM, 1999/ and /Olsson et al, 1994/.

Models:

Mathematical model (Swedish: Matematisk modell): Mathematical equations expressing the physical system together with the processes considered and including simplifying assumptions.

Conceptual model (Swedish: Begreppsmodell): A model which defines the geometric (or structural) framework in which the problem is to be solved, the size of the modelled volume (scale), the constitutive equations (mathematical model) for the processes included in the model and the boundary conditions. (In some literature “conceptual model” also includes what is here called “Descriptive model”.)

Interpretation model (Swedish: Tolkningsmodell): Chosen mathematical model for a specific interpretation that is valid for the concepts in question /e.g. Theis, 1935/.

Hydrogeological Descriptive model (Swedish: Hydrogeologisk modell): A geoscientific model, based on a specified conceptual model, with a limited extent and defined geometries of domains, in which the parameters are assigned to domains with a description of their spatial distribution and, finally defined boundary conditions /SKB, 2001b/.

Groundwater flow model (Swedish: Grundvattenflödesmodell): Application of the mathematical model to the hydrogeological descriptive model. The model may be analytical or represented by a computer code.

Groundwater modelling code (Swedish: Grundvattenmodelleringskod): The non-parameterised computer code used in groundwater modelling to represent a non-unique, simplified mathematical model of the physical framework, geometry, active processes and boundary conditions present in a reference subsurface hydrologic system.

Modelling:

Simulation (Swedish: Simulering): One complete execution of a groundwater modelling computer code, including input and output.

Model testing of a groundwater flow model (Swedish: Modeltest av en grundvatten-flödesmodell): Simulations of different major geometric alternatives or boundary conditions in an attempt to disprove a given geometric interpretation or boundary condition.

Calibration (Swedish: Kalibrering): The process of refining the model representation of the geometric framework, hydraulic properties and boundary conditions in order to achieve a desired degree of concordance between the model simulations and observations of the groundwater flow system.

Fidelity (Swedish: Riktighet): The degree to which a model application is designed to resemble the physical hydrogeological system. Calibration targets and acceptable residuals or residual statistics depend on the degree of fidelity chosen for a specific model application, which in turn depends on the objectives of the modelling project.

Sensitivity analysis (Swedish: Känslighetsanalys): A quantitative evaluation of the impact of variability or uncertainty in model inputs on the degree of calibration of a model (Calibration sensitivity analysis) and on its results or conclusions (Prediction sensitivity analysis).

Residual (Swedish: Rest, Residuum): The difference between the computed and observed values of a variable at a specific time and location.

Hydrologic condition (Swedish: Hydrologiska förhållanden): A set of initial conditions, boundary conditions and hydraulic properties applied to a defined geometric framework.

Boundary condition (Swedish: Randvillkor): A mathematical expression for the state of the physical system at the boundary that constrains the equations of the mathematical model. The boundary can be external or internal (e.g. tunnel).

Initial conditions (Swedish: Initialvillkor): A set of hydrologic conditions for a flow system, e.g. pressure distribution, that are distributed throughout the entire flow system at some particular time and that correspond to the antecedent hydrologic conditions in the aquifer system.

Parameter (*Swedish: Parameter):* Physical or chemical quantity (property, condition or state of the rock, soil (regolith), water courses, sea or atmosphere).

Stochastic (Swedish: Stokastisk): Consideration of parameters as random variables.

Effective hydraulic conductivity (Swedish: Effektiv hydraulisk konduktivitet): The effective hydraulic conductivity (K_{ef}) in the stochastic continuum theory represents the hydraulic conductivity value that will give the same specific discharge as an infinite statistically homogeneous domain under uniform, steady state flow for a given gradient /Rubin, 2003/. In this report it also represents the assumed constant value of a domain.

Block-effective hydraulic conductivity (Swedish: Blockeffektiv hydraulisk konduktivitet): (K_b) Value assigned to numerical grid-blocks. (Upscaled properties to blocks based on subgrid-scale heterogeneity) /Rubin, 2003/.

3 Concepts and parameters

The Geoscientific Site Descriptive models of a site should provide a quantitative description of the site and its surrounding area. The Geoscientific Site Descriptive models should also be of such detail and content as to provide sufficient geoscientific information about the site in terms of processes, geometric description, geometric element properties, initial and boundary conditions, thus enabling overall confidence that the models are adequate for their purpose. This chapter outlines concepts and data that are essential for the Hydrogeological Site Descriptive model.

Section 3.1 describes the purpose of the models and Section 3.2 outlines concepts and processes. In Section 3.3 the general mathematical formulations of the groundwater flow are described. Section 3.4 presents the geometric framework. and modelling scales. Section 3.5 some general points about the description scales used. In Sections 3.6 to 3.8 the parameters assigned to the geometric elements are discussed in more detail.

3.1 Purpose of the models

The hydrogeological descriptive model should provide data that are useful for modelling the advective flow in the groundwater system, including the density driven flow. More specifically, groundwater flow models should be able to calculate groundwater flow within a given volume under natural conditions (undisturbed) and with an open deep repository. For the open repository, the upconing of saline water, inflow to tunnels and drawdown, are important factors that should be modelled. In the undisturbed system, the flow paths within the modelled volume are important for the hydrogeochemical interpretation, while the flow paths from the repository area to discharge areas are important for Safety Assessment. The shoreline displacement must also be taken into account when modelling the long-time evolution of the groundwater flow.

3.2 Concepts and processes

The rock and soil is divided into domains with similar properties. Large deformations zones and soil layers form domains, which are illustrated in Figures 3-1 to 3-3. It is assumed that large deformations zones can be identified and included deterministically in the Site Descriptive model. The rock mass between the large deformations zones may be divided into different domains if properties differ significantly. The large deformations zones may also be divided into different domains if properties differ significantly.

The soil is modelled as Continuum Porous Medium. Two main concepts are used for property description of the rock; Discrete Fracture Network (DFN) and a Continuum Porous Medium (C). The properties may be assumed to be constant or stochastically distributed within the domains. The rock mass is generally modelled stochastically as Stochastic Continuum (SC) or with stochastic properties of the DFN, see Figure 3-4.

Saturated variable-density flow is modelled assuming that friction loss is constant. The ultimate driving force behind the saturated groundwater flow is the water table, which depends on the precipitation rate and the hydraulic properties of rock and soil.

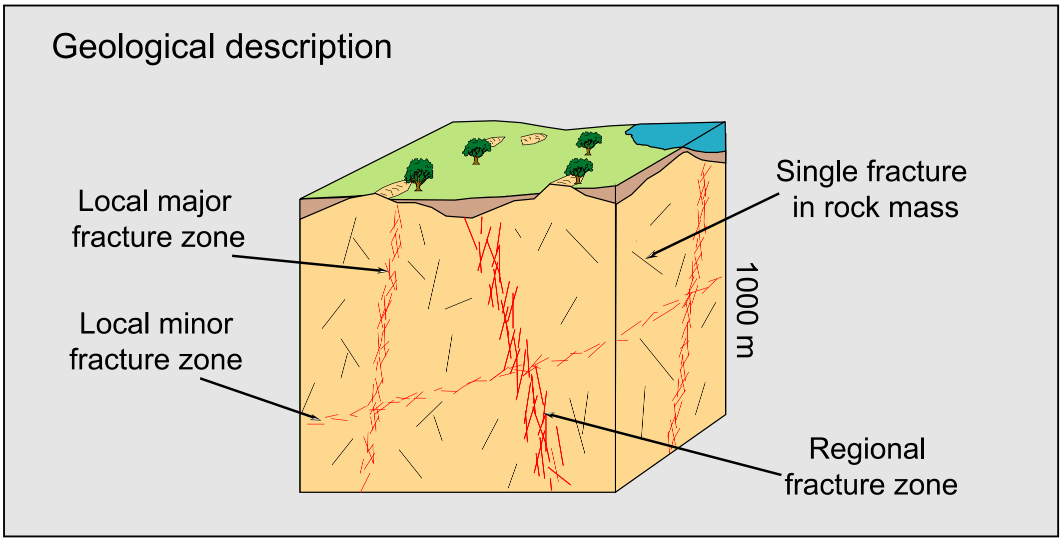


Figure 3-1. *Illustration of the principal features in a geological model.*

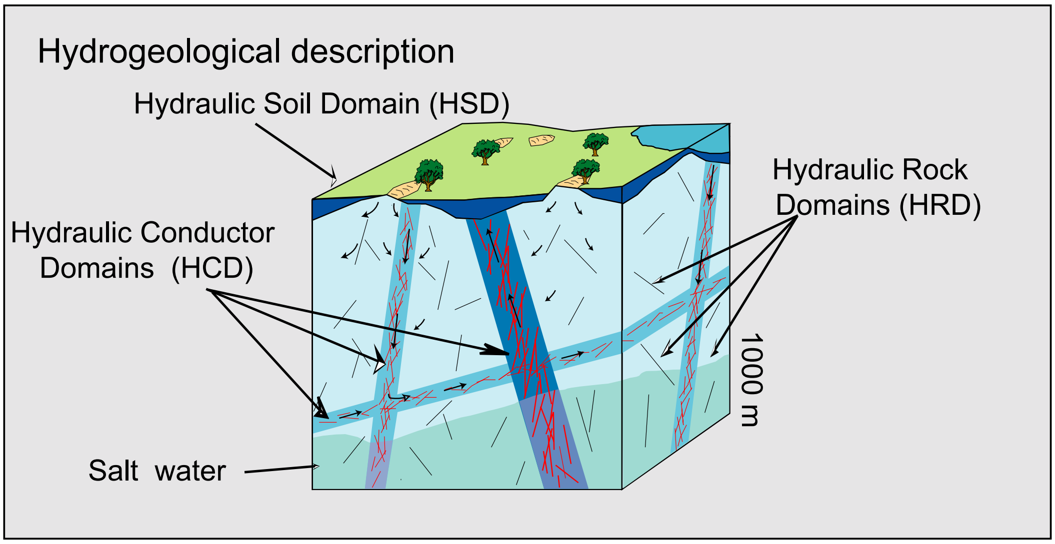


Figure 3-2. *Illustration of the principal features in a hydrogeological model.*

Dynamic modelling of the detailed surface hydrology (modelling of flows in water courses and the unsaturated flow in soil) may be considered in future modelling but is not considered essential for the large scale groundwater flow modelling.

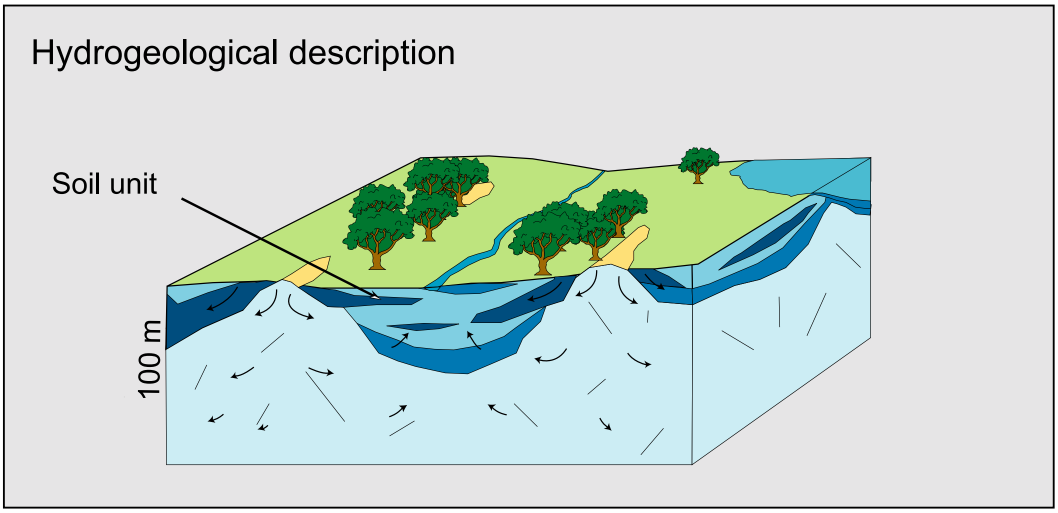


Figure 3-3. Illustration of the principal features close to surface in a hydrogeological model.

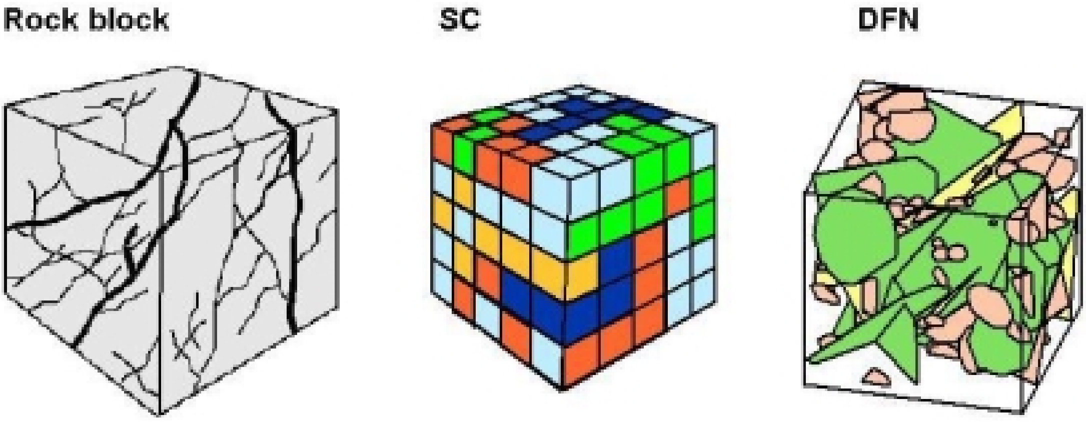


Figure 3-4. Schematic view of the stochastic continuum (SC) and the discrete fracture network (DFN) modelleling approaches.

3.3 Mathematical model

The parameterisation of the groundwater flow models based on the DFN (Discrete Fracture Network) or C (Continuum) or SC (Stochastic Continuum) concepts is slightly different but in principle the same equations are used as for calculation of the advective flow. The basic advective flow equations including density driven flow are as follows:

Equation of motion:

$$q = -\frac{k}{\mu} \cdot \left(grad(p) + \rho \cdot g \cdot grad(z) \right) \tag{3-1}$$

The continuity equation (mass conservation) is given by:

$$div(\rho \cdot q) + \frac{d(\rho \cdot n)}{dt} + \rho \cdot Q = 0 \qquad (3\text{-}2)$$

Transport equation:

$$div(D\rho \cdot grad(C) - C\rho \cdot q) = \frac{\partial(\rho n_e C)}{\partial t} + Q\rho \cdot C_s \qquad (3\text{-}3)$$

The equations of state are:

$$\rho = f(T, C, p) \qquad (3\text{-}4)$$

$$\mu = f(T, C, p) \qquad (3\text{-}5)$$

Advective flow mean velocity (average linear velocity):

$$\mathrm{v}_a = \frac{\mathrm{q}}{n_e} \qquad (3\text{-}6)$$

(q: flow per unit area (specific discharge), *k*: permeability, μ: dynamic viscosity, *p*: water pressure, ρ: fluid density, *g*: acceleration of gravity, *z*: elevation, n_e: Kinematic porosity or transport porosity, *n*: Total porosity Q: withdrawn (injected if negative) flow per unit of volume, *t*: time, *T*: temperature, *D*: Dispersion tensor, *C*: mass fraction of soluble species (mainly salt), C_S: Mass fraction injected/withdrawn fluid).

As can be seen in the equations, a few transport parameters (Dispersion coefficient (Hydrodynamic dispersion and diffusion), kinematic flow porosity) are necessary for the conservative transport of salt. The concepts of how the porosity is distributed in crystalline rock (matrix porosity, fracture-filling porosity, kinematic porosity and total porosity (volume) of fracture) are described by /Berglund and Selroos, 2003/ and need not be further elaborated upon here.

The above equations form the basis for calculating water flow, taking into account pressure, temperature and density conditions. The permeability is given by the pore system properties while the dynamic viscosity determines the fluid properties. Groundwater flow simulations will to some extent be based on permeability etc, including the effects of primary salinity and temperature. However, the density effect may be disregarded for some simulations and can generally be omitted when interpreting the hydraulic properties from hydraulic tests. If the density effect is disregarded, the above equation can be simplified as below.

The flow vector is composed of a pressure gradient *(grad (p))* and a gradient which is dependent on the forces of gravity (*ρg grad(z)*). Providing the water has constant density, the equations are expressed as follows:

Equation of motion:

$$q = -\frac{k \cdot \rho \cdot g}{\mu} \cdot grad\left(\frac{p}{\rho \cdot g} + z\right) = -K \cdot grad\left(\frac{p}{\rho \cdot g} + z\right) = -K \cdot grad(h) = K \cdot i \qquad (3\text{-}7)$$

The continuity equation:

$$-div(q) \approx \frac{S_S}{\rho \cdot g}\frac{d(p)}{dt} + Q \approx S_S \frac{d(h)}{dt} + Q \qquad (3\text{-}8)$$

$$K = k \cdot \frac{\rho_w \cdot g}{\mu_w} \qquad (3\text{-}9)$$

$$S_s = (\alpha + n \cdot \beta) \cdot \rho_w \cdot g = n \cdot c_t \cdot \rho_w \cdot g \qquad (3\text{-}10)$$

(Hydraulic conductivity (K), Specific storage coefficient (S_s). In groundwater literature, the system compressibility c_t corresponds as follows; $c_t = \alpha/n+\beta_w$. α: Compressibility coefficient of a porous medium, β_w: compressibility of water).

In a DFN model 2D features are spatially interconnected. The primary parameters for these 2D features assuming constant fluid properties are transmissivity (T) and Storage coefficient (S).

The storage capacity of the system can exhibit local variations, depending on the effective rock stress and if the system is confined or unconfined. The effect of an unconfined part of a groundwater flow model is a delayed pressure response in part of the model. The parameter to consider here is the Specific yield (S_y) that will be included in the simulations if deemed relevant. The effect of the effective stress will not be included in the large-scale Site description modelling.

At present unsaturated flow is not considered, and a simplified approach is therefore used in the groundwater flow simulations. If the unsaturated flow is modelled, the primary data for estimating the soil-water retention and capillary conductivity curves will be the geological description of the soil deposits with their grain-size distribution curves.

3.3.1 Fluid independent parameters

The parameters of the porous medium in groundwater hydraulics are Hydraulic conductivity (K), Transmissivity (T), Specific storage coefficient (S_s), Storage coefficient (S), Specific yield (S_y) (or Apparent specific yield, S_{ya}) and Specific retention (S_r). (Theoretically $n=S_y+S_r$ but in field tests (free drainage of the porous system) the volume of water drained can be less than expected due to trapped gas in the porous system; $S_{ya} \leq S_y$.). It is generally assumed that that temperature, pressure and concentration of solutes have a negligible effect on these paramerers and thus the groundwater flow. If temperature, pressure and solute concentration have a significant impact on the groundwater flow, fluid independent properties of the rock and surficial deposits should be used; *k: intrinsic permeability, n: total porosity,* c_t*:(total) system compressibility.*

The total porosity cannot be estimated in hydraulic tests, although the product of n and c_t can be calculated if the density and acceleration of gravity are known. Therefore, a *Porosity-compressibility-factor* (nc_t), *(1/Pa)* can be defined.

For 2D domains the convention in petroleum engineering is the *Permeability-thickness product (kb),* (m^3), integrating over the thickness b. In the same way the storage capacity should be termed *Porosity-compressibility-thickness product* (nc_tb), *(m/Pa).* For a fracture it is more relevant to just define 2D fluid independent parameters with a notation not indicating integration over a thickness as above. An alternative can be *intrinsic transmissivity (iT*) and *intrinsic storage coefficient (iS).*

The influence of temperature, TDS and water pressure on the evaluated hydraulic properties will be made. If considered relevant the analysis of the hydraulic properties can be made on fluid independent properties, as for example intrinsic permeability (k), and applied in the groundwater flow simulations with assumed or simulated temperature distributions within the rock mass.

For each hydraulic test in boreholes representative fluid properties estimated for the test section; density (ρ_W) and dynamic viscosity (μ_W). These properties are calculated from water temperature, TDS and water pressure. Estimate of TDS is generally based on Electrical Conductivity (EC) of the water. A Fluid Coefficient for intrinsic permeability (FC_T) and porosity-compressibility-product (FC_S) can be set up as:

$$FC_T = \frac{\rho_w \cdot g}{\mu_w}$$

$$FC_S = \rho_w \cdot g$$

3.4 Geometric framework

3.4.1 Size of descriptive models

As pointed out in the text above, the planning envisages a *Regional Site model* and *Local Site model*. Region Site model description is the base for a regional groundwater flow model that should provide boundary conditions for the Local Site model. The size of the Regional Site model should be large enough so its boundary conditions should not have a large influence of the hydraulic conditions at the Local Site model boundary. The Local Site model should be large enough to cover the deep repository and the near surroundings to the deep repository for the detailed modelling of the groundwater flow field.

The Local Site model is expected to cover some 10 km^2 and the Regional Site Model a much larger area. Site Investigations will be performed within these areas, and the intensity of investigations within the Local Site area will be greater, as the site descriptive model demands less uncertainty. “Super Regional models” may also be made to support the discussion of appropriate boundary conditions for the Regional Groundwater flow models. Such models are based on the existing knowledge of geology and hydrogeology within the modelled area. Figure 3-5 illustrates the Regional and Local Site model areas in Simpevarp as defined winter 2003.

3.4.2 Modelled domains

The geometric framework is common to all disciplines. The investigations carried out by the different disciplines may serve as a basis for independent evidence or support the interpretation of the geometric framework as well as initial and boundary conditions. Therefore, the integrated evaluation of data is essential.

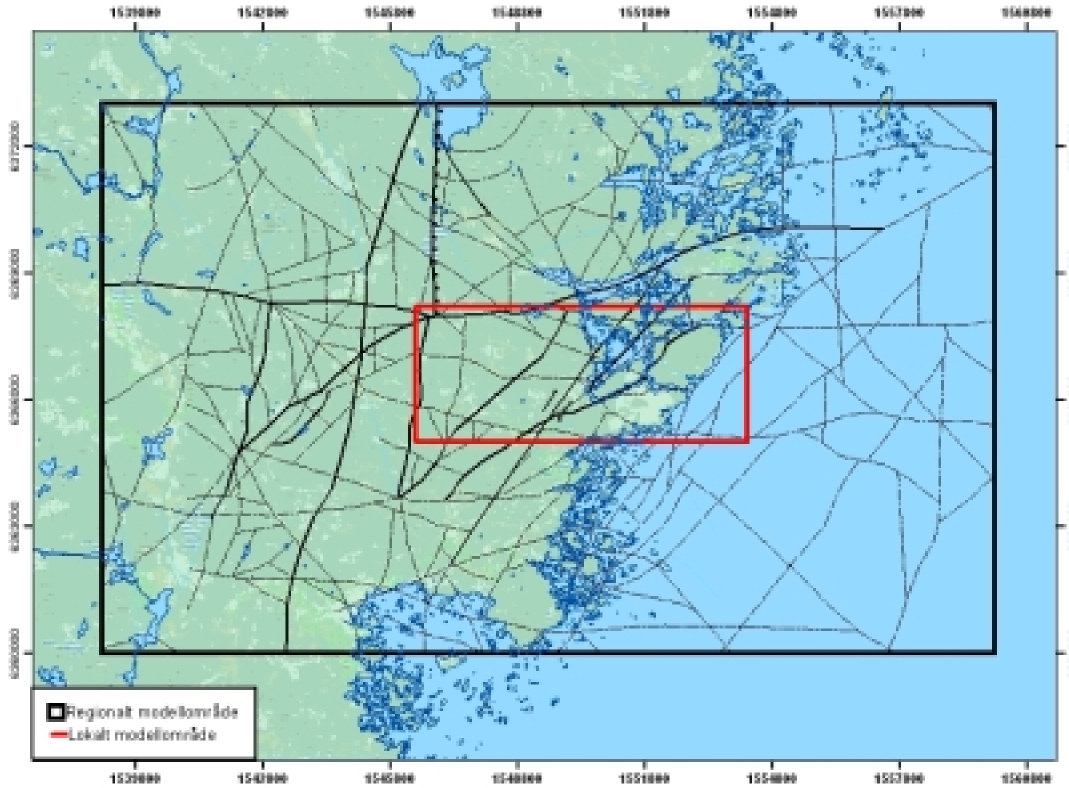


***Figure 3-5.** The Regional (black) and Local Site (red) model areas in Simpevarp as defined winter 2003.*

The geoscientific descriptive site model is divided into geometric units based on the differences in properties. The differences should be significant in some respect for the model and its use. As pointed out in /SKB, 2000, 2001b/ the Design and Safety Assessment disciplines are the main users of geoscientific descriptive models.

The Geological model is the basis for all descriptive models of the site. Figure 3-1 shows the main geological elements. Of primary interest are large *deformation zones* that may have an impact on several of the geoscientific descriptive models. These large deformation zones (Generally termed; *Regional fracture zones* and *Local major fracture zones*, see /SKB, 2000/) are therefore important geometric units to be defined in space. Some *Local minor fracture zones* will be defined in space (increasingly so as the investigations proceeds) but most of them will be considered as stochastic distributions within the modelled volume as it is not possible to define them all by investigations. *Fractures* will also be considered as stochastic distributions within the modelled volume. These stochstic distributions are based on observations (defined in space) on outcrops and in boreholes. Depending on the properties of the rock mass (such as rock type, mechanical properties etc) of the modelled rock volume, *Rock Units* and *Rock Domains* are defined within the model, see Figure 2-1.

The analysis of the hydraulic single-hole tests and interference tests together with the geometric description of the deformation zones and the rock units results in the properties assigned to geometric units and termed *Hydraulic Conductor Domains (HCD)* and *Hydraulic Rock Domains (HRD),* see Figures 2-2 and 3-2.

The geological descriptive model also includes a model of the soil deposits, mainly quaternary deposits, with deposit types and their stratification. Based on the geological model and the hydrogeological investigations and evaluations, the soil deposits are divided into *Hydraulic Soil Domains (HSD*), see Figure 3-3.

3.5 Description scale

Parameter values in the Descriptive models should be linked to a description scale or spatial resolution required by the user, who are primarily the Design and SA functions /Andersson, 2003/. A detailed description is needed for the models describing the solute transport from the canisters and the design of the deposition tunnels and deposition holes. The design of the transport tunnels and the modelling of flow field near the deep repository require less detailed description than near the deposition tunnels. For large-scale models providing boundary conditions to Local Site Scale models large description scales are useful and sufficient.

For a spatially varying property, the scale is the size of the domain over which properties are averaged, the *description scale*. Different applications may have different requirements in respect of description scales. In a general sense, the geoscientific description covers minor as well as large features within the entire regional modelling volume but the uncertainty in the description of minor features is generally greater further away from the deep repository due to less detailed investigations. This means that the descriptive model requirements of Local Site models and Regional Site models are different in terms of uncertainty but also in terms of the justification for using a larger description scale.

The description scales chosen are the 5 m scale (approximately canister size), the 20 m scale (tunnel size) and the 100 m scale (Regional Site Descriptive modelling) see Figure 3-6. The 5 m scale is intended for the description of the near field of the canisters and deposition tunnels. The 20 m scale is chosen for the local model covering the repository volume. The 100 m scale is for description and modelling in the regional scale. The descriptions scales above have considered relevant for the different types of modelling that will be made for each site.

However, some of the hydraulic tests performed are intended to give a description scale of less than 5 m. The conductive fracture frequency is intended to be described down to dm-scale. Those data will be useful for the near-field modelling and comparison to the 5 m scale.

Although most parameters are associated with a description scale, some parts of the geoscientific description can be considered more or less scale-independent, such as the size distribution of fractures, though restricted to the minimum observation size and observation window of the entire sample.

In hydrogeology the different description scales are linked to the measurement scale, see below. The quantification from field measurements may represent effective (average) values for different size volumes, depending on the investigation method and duration of tests. Measurements are made with different resolutions in space, here termed *measurement scale*. In boreholes the measurement scale is normally the length of the tested section

As the averaging process for permeability is not straightforward, different measurement scales and test times facilitate analysis of the averaging process and testing of models with different description scales.

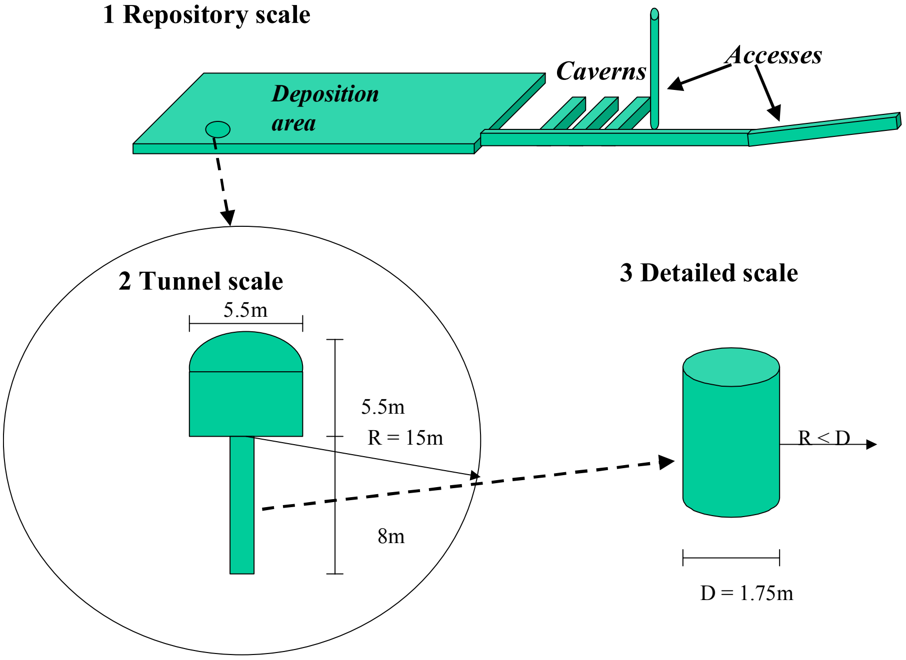


Figure 3-6. *Schematic illustration of the description scales /after Andersson et al, 2002b/.*

3.6 Hydraulic properties of hydraulic domains

In this section the assignment of properties to the hydraulic domains is presented in more detail. Generally the hydraulic domains correspond directly to the defined geological domains. However, if the hydraulic properties vary significantly within a geological domain it may be divided into several hydraulic domains. The opposite is also possible; several geological domains may be merged into one hydraulic domain if the hydraulic properties do not vary significantly.

Transport properties relevant to salinity are not included below as they are presented in /Berglund and Selroos, 2003/. However, results from hydraulic tests and tracer tests may be used to establish a correlation model for the spatial assignment of kinematic porosity to the hydraulic domains.

The large deterministic deformation zones here called Hydraulic Conductor domains may have a low permeability and rather act as hydraulic barriers than conductors. However we have chosen to call all large deterministic deformation zones for Hydraulic Conductor domains and the property description tells whether a HCD is a conductor or act as a barrier.

3.6.1 Hydraulic Conductor domains (HCD)

HCDs consist of one or several surfaces of a defined thickness. The parameters for each HCD are defined in Table 3-1 and Figure 3-7.

Table 3-1. HCD Parameters.

Parameter	Notation	Unit	Description scale (m)	Spatial representation	Comment
Transmissivity	T	m^2/s	10–100	Constant or stochastic distribution within HCD.	One deformation zone may consist of several HCDs.
Storage coefficient	S	–	10–100	Constant or stochastic distribution within HCD. Generally assumed to be a function of T.	Interference tests are used. Generally difficult to estimate from tests because of geometric complexity and long distances between pumped section and observation sections.
Total width of zone (Formation thickness)	b	m	–	Constant within each domain.	Is based on interpretation of geological, hydrogeological and geophysical data from boreholes and surface mapping.

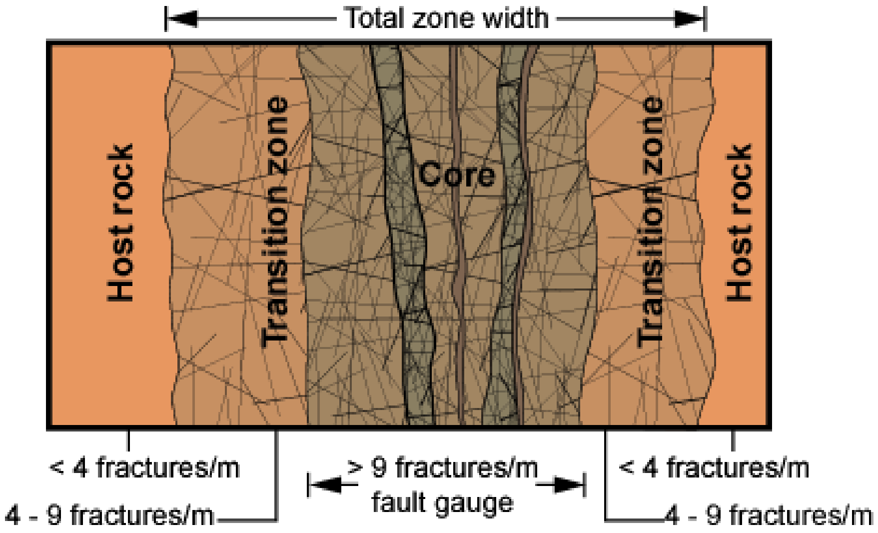


Figure 3-7. Schematic illustration of the structure of a brittle deformation zone /Munier et al, 2003/.

A HCD is generally considered to be a hydraulic feature with constant properties and a constant thickness (b), which is based on the geological estimate of the average total deformation zone thickness, see Figure 3-7. One deterministic deformation zone may be divided into several domains if data indicate spatial differences deemed to be of significance for the simulations. The extent of a HCD's surface(s) is generally several 100 m and the evaluated properties are normally average values representing description scale between 10 and 100 m, at least when the HCD is fairly permeable.

The HCD hydraulic feature may have a complex internal structure which varies from relatively few large interconnected fractures to a fracture zone with differences in fracture intensity and fracture filling, as indicated in Figure 3-7. This complexity is not considered , at least initially, but a stochastic distribution of the properties in a medium-large scale (10–100 m) may be used as an alternative to constant values. Tests may be performed on the behaviour of a HCD model with a high discretisation and fracture network (see next section for parametrization of DFN) in order to obtain a better understanding of how to assign average properties in the 100 m scale. The geological classification may justify defining classes of internal heterogeneity of deformation zones that can form the basis for assigning more elaborate properties that can be useful for hydrogeology as well as for transport.

Deformation zones may have a low-conductive core (clay filled) zone with more conductive parts in the rest of the core and the transition zone. In such cases the HCD is anisotropic and must be considered when implemented in the groundwater flow model.

Storage parameters are difficult to estimate. However, the results of tests carried out during the construction of Äspö HRL /Rhen et al, 1997c/ and from projects performed at Äspö HRL /e.g. Rhen and Forsmark, 2001/ show a correlation between T and S that can be updated as new information is gathered during Site Investigations. If the storage of a HCD reaching ground surface is to be modelled more exactly, the drainage of the fracture system at surface should be included when pressure decreases below atmospheric level. In this case the storage coefficient should be somewhat less than the estimated total porosity of the HCD.

3.6.2 Hydraulic Rock Domains (HRD)

HRD consists of one or several rock units outside the defined HCDs. The parameters for each HRD are defined in Table 3-2 or 3-3. A HRD may be described as having constant properties but generally the properties are assumed to be stochastically distributed. Two main approaches are used for the modelling of HRDs: The Discrete Fracture Network model (DFN model) and a Continuum Porous Medium model or Continuum model (C model). These approaches are discussed below.

The base case consists of hydraulic features described by:

- Sets of hydraulic features (with different properties).
- The following are defined for each set:
  - Orientation distribution.
  - Size distribution.
  - Intensity (P_{32}, Fracture area/volume).
  - Spatial model of the centre of a hydraulic feature.
  - The shape of the feature. Generally assumed to be circular or quadratic.
  - Transmissivity distribution (and distributions for other properties if needed).

Table 3-2. Parameters for the HRD – DFN approach.

Parameter	Notation	Unit	Description scale (m)	Spatial representation	Comment
Transmissivity	T	m^2/s	(1–100)	Stochastic distribution within HRD.	
Storage coefficient	S	–	(1–100)	Stochastic distribution within HRD. Generally assumed to be a function of T.	Interference tests are used. Generally difficult to estimate from tests because of geometric complexity and long distances between pumped section and observation sections.
Total width of feature (Formation thickness)	b	m	–	Constant within each feature. Generally assumed to be a function of T.	Is based on the interpretation of geological, hydrogeological and geophysical data from boreholes and surface mapping.

This description applies to groundwater flow modelling with DFN codes but also to input data for the pre-processing of the transmissivity field to obtain a hydraulic conductivity field in the form of a continuum code, such as the previously mentioned DarcyTools (Mixed DFN-Continuum approach (MDC)). In principle, the description scale is scale-independent. However, a decision must be made in context of the actual problem how to perform stochastic simulation of the large features, taking into account the size of the HCDs, and how small features should be simulated in terms of the numerical discretisation (grid size). Results from /Andersson et al, 2002a/ and /Rhén et al, 1997/ indicate that the maximum size (radius) of the stochastic hydraulic features may be around 500 m (due to the defined HCDs) with the minimum trace lengths of mapped fractures about 1 m. In continuum codes using DFN for the generation of properties, sub-grid features may be taken into account by adding sub-grid values, as constants or distributions, to each cell if relevant. The properties within each hydraulic feature are generally assumed to be constant. However, a small-scale hydraulic feature should be considered to be a single fracture while large-scale hydraulic features are likely to be fracture zones (local minor fracture zones), thus an interconnected network of fractures. The spatial assignment method described above is the main method that will be used.

Table 3-3. Parameters for HRD – SC approach.

Parameter	Notation	Unit	Description scale (m)	Spatial representation	Comment
Hydraulic conductivity	K	m/s	5, 20, 100	Constant or stochastic distribution within HRD.	
Specific storage coefficient	S_S	1/m	(5, 20, 100)	Constant or stochastic distribution within HRD. Generally assumed to be a function of K.	Interference tests are used. Generally difficult to estimate from tests because of geometric complexity and long distances between pumped section and observation sections.
Specific yield	S_y	–	(100)	Constant or stochastic distribution within HRD.	Interference tests are used. Generally difficult to estimate for low conductive formations.

There are several other options for the spatial assignment in a Continuum model. Constant hydraulic conductivity can also be assigned to an HRD and should be termed effective hydraulic conductivity (K_{ef}). In fractured media it may be questionable as to whether one can obtain a stable mean K by integration over a large bedrock volume as proposed in the stochastic continuum theory. However, it is useful to estimate K_{ef} from tests with different measurement scales and then test the groundwater flow model against measurements in order to calibrate K_{ef}.

The spatial assignment of the stochastic field in a Stochastic Continuum model (SC model) may also be carried out in several ways. An alternative that has been used in /Rhén et al, 1997c; Walker et al, 1997/ and /SR 97, 1999/ is the establishment of the empirical relation of hydraulic conductivity based on the measurement scale in order to scale the mean and the standard deviation to the grid size used for block-effective hydraulic conductivity (K_b). In these cases no spatial correlation was assumed.

Geostatistics can be used to analyse the data and establish spatial correlation models that are then used for simulation of the stochastic field of properties in space /Isaaks and Srivastava, 1989; Deutsch and Journel, 1997; Jensen et al, 2000; Deutsch, 2002/. Geostatistics is frequently used within the field of Petroleum Engineering, mostly in respect of porous mediums. /Jensen et al, 2000/ highlight the fact that research on the geostatistical treatment of permeability data is still needed, as it is not obvious that the basic assumptions made are fully justified. In a highly heterogeneous medium such as fractured crystalline rock, this is even more questionable. Classical permeability treatment, such as injection tests at rather long distances also give correlation models with high nugget /Niemi, 1995; La Point, 1994/, which in practice then give a more or less uncorrelated field when simulating the properties. However, relevant correlation models of Stochastic Continuum models can probably be obtained by transferring DFN to a fine-grid SC model and applying the geostatistics to the grid values (Hoch et al in /SKB, 1998/).

3.6.3 Hydraulic Soil Domains (HSD)

The Geological model of the soil deposits and hydraulic tests in soil deposit form the base for the hydrogeological model of the soil layers. Soil units, which are considered to have significantly different hydraulic properties, form Hydraulic Soil Domains (HSD) with specified hydraulic properties. HSD consists of one or several soil units. The parameters for each HSD are defined in Table 3-4. Topography and bedrock surface defines the total soil depth and is thus essential for the modelling of the HSD.

Table 3-4. Parameters for HSD.

Parameter	Notation	Unit	Description scale	Spatial representation	Comment
Hydraulic conductivity	K	m/s	(1–100)	Constant or stochastic distribution within HSD.	Based on particle size analysis and hydraulic tests.
Specific storage coefficient	S_S	1/m	(1–100)	Constant or stochastic distribution within HSD.	Interference tests are used. Generally difficult to estimate for low conductive formations.
Specific yield	S_y	–	(100)	Constant or stochastic distribution within HSD.	Interference tests are used. Generally difficult to estimate for low conductive formations.

As base case, constant parameter values are assigned to each defined HSD. The available data are too limited for the construction of a spatial model of the properties of each domain, and is not considered essential. A rough spatial model may possibly be made to test the effect on, for example, discharge area behaviour.

Storage parameters are difficult to estimate. However, there are results in the literature and from other projects that can be used and then updated as new information is gathered during Site Investigations.

3.7 Surface hydrology

3.7.1 General

The main geometric elements in surface hydrology are lakes, watercourses and topography. Topography defines *surface-water divides* and *catchment (drainage) areas*. Generally one can expect groundwater divides to coincide with surface-water divides. *Precipitation* minus *evapotranspiration* (*=effective precipitation*) on land surfaces, lakes and watercourses gives the net flow in the watercourses, the *runoff*, and the subsea outflow of groundwater (if a catchment area is bounded by the sea). On land surfaces, part of the effective precipitation flows as *overland flow* (flows on the land surface) and *interflow* (part of the infiltrating water that flows beneath the surface but above the saturation zone) directly into the lakes or watercourses. Interflow may also emerge as seepage at surface and continue as overland flow to streams (some times called *throughflow* and the overland flow is then called *return flow*). The rest of the infiltrating water, the *net infiltration*, *percolates* through the *unsaturated zone* and *recharges* the groundwater in the *recharge areas*. An area where subsurface water is *discharged* to the land surface, to bodies of surface water or to the atmosphere is called a *discharge area*. The saturated flow from groundwater to surface water is called *baseflow* (*base-flow recession* is used when evaluating flow rate component in streams emanating from saturated groundwater flow in stream hydrographs) and to seawater *subsea outflow*. *Runoff* from a catchment area is an important variable in hydrogeology. *Mean effective precipitation* can be estimated for a catchment area by dividing the runoff by the catchment area, which sometimes is termed *Specific runoff.* (The terms used above are the standard terms for describing surface hydrology).

All factors above are essential for the estimation of appropriate upper boundary conditions for the groundwater flow model. The near-surface geology typical for the sites that are investigated and groundwater flow is illustrated in Figure 3-8.

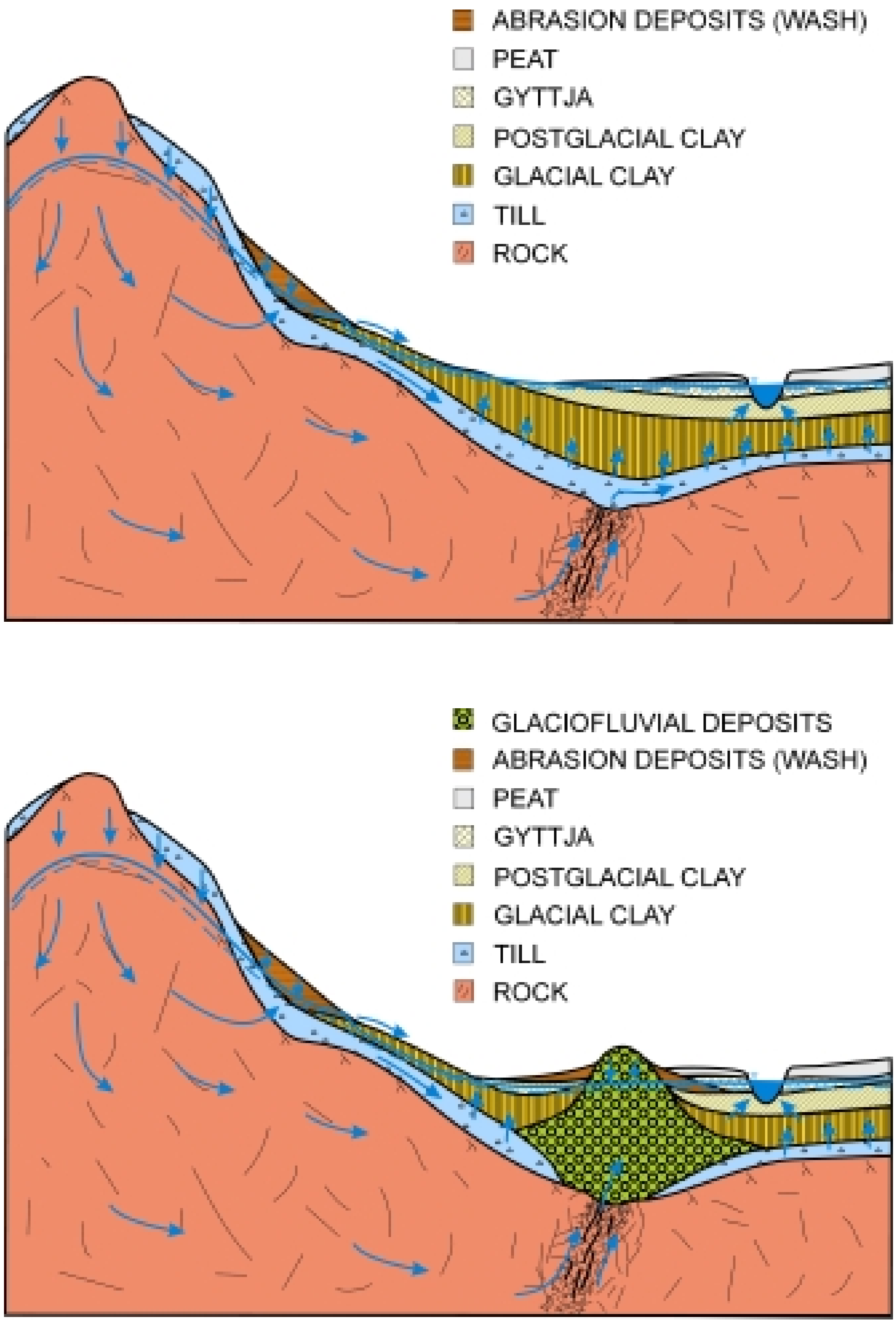


Figure 3-8. *Illustration of the geology and groundwater flow close to surface. Top: Till overlain by clay, gyttja, peat and abrasion deposits is expected in large part of the investigated areas. Bottom: In some part of the investigated areas glaciofluvial deposits in form of eskers can be found. (Vertical exaggeration approximately 20:1).*

3.7.2 Topography

Topography is essential for the definition of catchment areas for water balance (hydrological budget) calculations and as a geometric element in the simulations.

3.7.3 Watercourses, lakes and sea

The geometry of watercourses, lakes and the sea in the vicinity of the investigated site are simulation elements as these are the primary discharge areas but may also act as recharge areas under certain hydraulic conditions. Of primary interests are the annual mean and temporal distribution of water levels in watercourses, lakes and sea as well as runoff rates in the watercourses.

3.7.4 Meteorological conditions

The annual mean and the spatial and temporal distribution of precipitation, potential evapotranspiration, air temperature and the presence of a snow cover are important for assessing the upper boundary conditions and making comparisons with runoff estimates.

3.7.5 Overland flow, interflow and groundwater recharge

The geological model is the base for describing the factors leading to the occurrence of overland flow and interflow, although runoff rates and the meteorological variables are used for the quantification of the flows in the water balance. Details of overland flow and interflow are not considered important. However, the upper most part of the soil (regolith), 0.5–1 m below surface, generally has a much higher hydraulic conductivity than deeper lying regolith, which strongly affects the interflow and the groundwater flow when the level of the water table is close to surface.

The effect of the recharge as responses in the geosphere can be gauged by measuring the level of the water table, the piezometric levels in wells with observation sections at different depths in soil and rock as well as levels in lakes, watercourses and sea. Monitoring along a few sections crossing valleys, with for the regional typical geological settings, will be useful for understanding and semi-quantification of the of the near-surface flow in recharge and discharge areas. Observations of the vegetation and springs will also reveal discharge areas and some of the hydrogeological conditions.

Generally the (natural) water table can be expected to follow the topography with the largest depths to the water table at the highest topographic points. However, the spatial variability of the level of the water table and piezometric levels in the rock can be expected to be significant due to the heterogeneity of the rock in areas with thin soil (regolith) cover. This will probably be most pronounced at the highest topographic points.

3.8 Boundary and initial conditions

Generally the assigned boundary conditions may be of five types:

- Specified head (pressure) boundary (Dirichlet condition).
- Specified flow boundary (Neumann condition).
- Head- (pressure-) dependent flow boundaries (Cauchy or mixed boundary condition).
- Free-Surface boundary (Head equal to the elevation of the boundary, e.g the water table).
- Seepage-Face boundary (Similar to Free-Surface boundary).

Different boundary conditions are assigned due to the position of the boundary and the conditions related to the problem under study.

The upper boundary is modelled with somewhat simplified boundary conditions, as is often the case with simulations. The runoff rate is used to estimate the average effective precipitation rate. Precipitation and evapotranspiration rates are important for the interpretation of some site-specific data and may also be used for more detailed modelling of the near-surface flows. External sources such as pumping or infiltration must also be identified and included in the simulations. Water level measurements in open boreholes are normally used for calibration of the groundwater flow model.

Table 3-5. Parameters for surface boundary conditions.

Parameter	Notation	Unit	Scale	Spatial representation	Comment
Precipitation	P	mm/y, mm/d	(10 km)	Constant or variable over time. Spatial distribution if required.	
Potential evapotranspiration	ET	mm/y, mm/d	(10 km)	Constant or variable over time. Spatial distribution if required.	
Surface water and sea water level	h	m	–	Constant or variable over time.	
Salinity	TDS	mg/L	–	Constant or variable over time.	Salinity in the sea.
Runoff	Q_R	m^3/s	(1–10 km)	Constant or variable over time.	Runoff rates are estimated or measured for larger catchment areas.
Pump rate	Q_P	m^3/s	–	Constant or variable over time.	
Infiltation rate	Q_I	m^3/s	–	Constant or variable over time.	

The vertical boundaries generally have different boundary conditions due to their location and depth below ground- or sea level. In the regional model it is of importance to define the modelling volume so that boundary conditions can be described in as simple and trustworthy a fashion as possible. The position and spatial distribution of boundary conditions are decided based on available data concerning pressure and TDS distributions in boreholes, topography and the geological description. For Local Site model the boundary conditions are generally taken from a Regional Site model. The bottom boundary in the Regional Site model is assumed to be a no-flow boundary as the depth to the bottom is so great that it has a very limited influence on the flow field at repository depth.

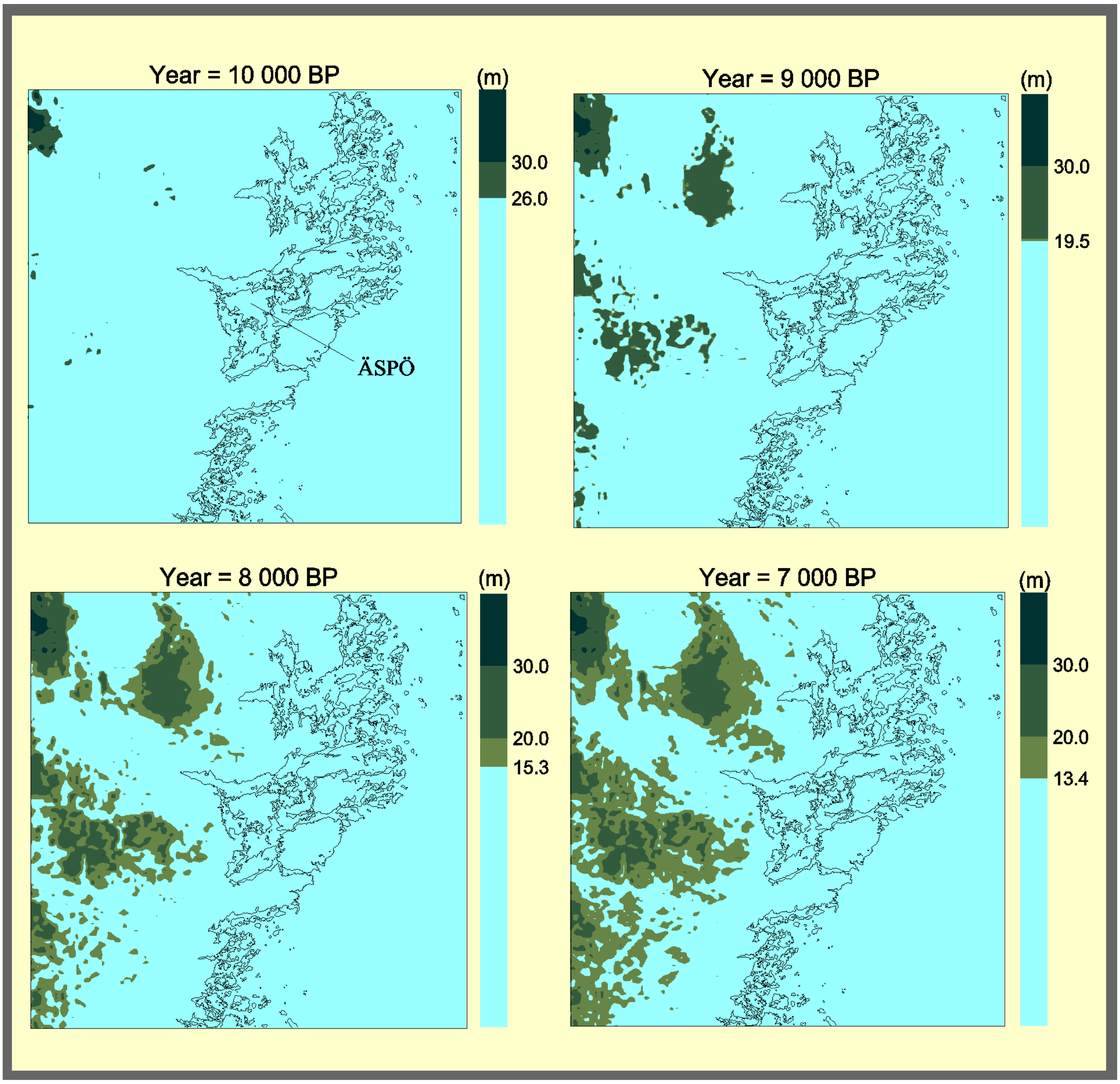
Table 3-6. Parameters for vertical and bottom boundary conditions.

Parameter	Notation	Unit	Scale	Spatial representation	Comment
Pressure	p	kPa	(10–100 m)	Constant or variable over time.	Difficult to assess more exactly from measurements.
Salinity	TDS	mg/L	(10–100 m)	Constant or variable over time.	Difficult to assess more exactly from measurements.
Specific discharge	q	m/s	(10–100 m)	Constant or variable over time.	A model parameter.

Initial conditions must be specified for transient simulations. If the task is to simulate interference tests, a stationary simulation with the present and undisturbed boundary conditions is probably adequate. Such a stationary simulation is based on a calibrated groundwater flow model. Groundwater flow modelling is described in Chapter 6.

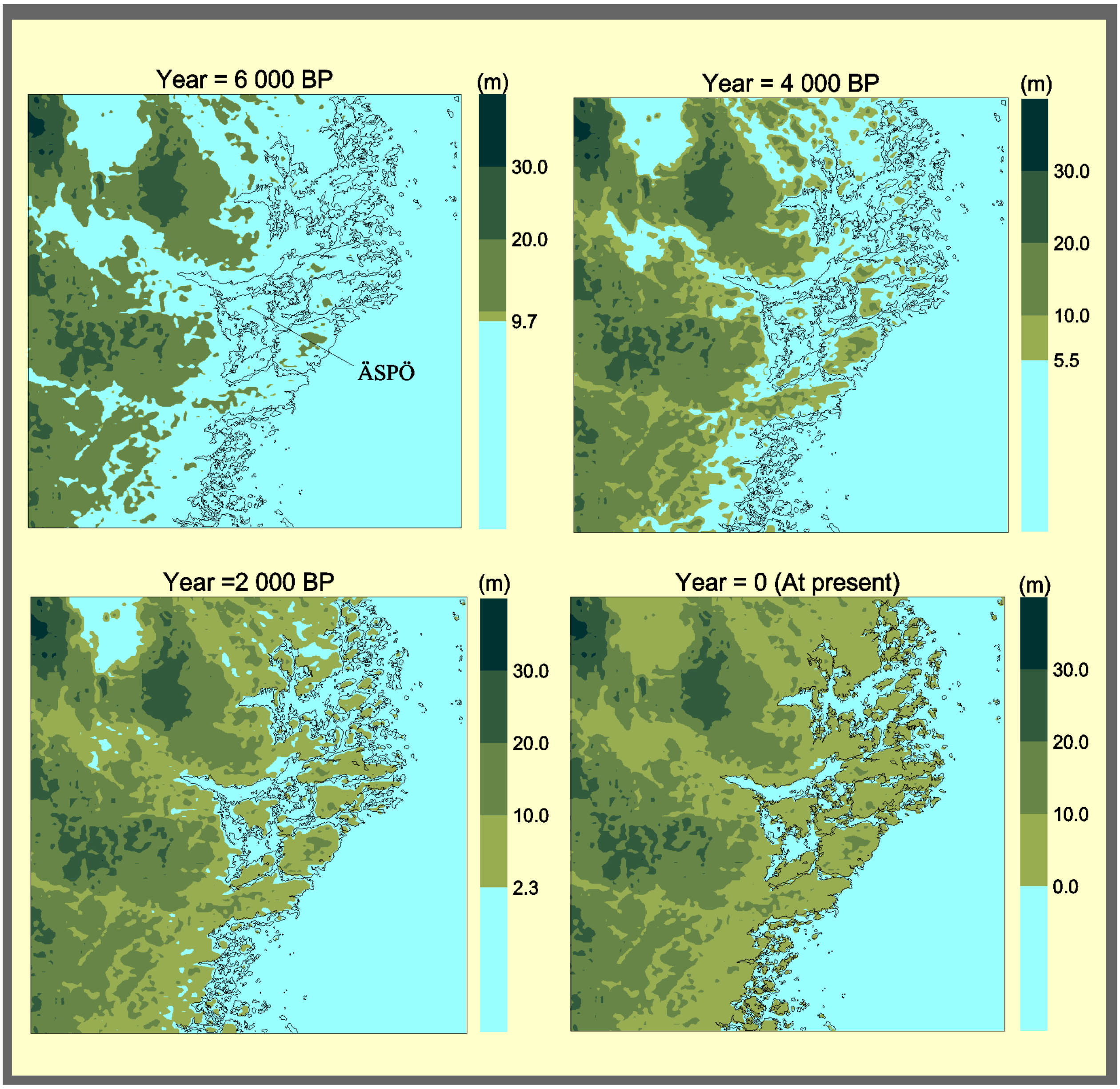
Pressure observations may be important for the understanding the flow system in recharge and discharge areas.

Time dependent boundary conditions have to be considered for some groundwater flow simulations. The long-term groundwater flow simulations have to consider the shore displacement that is illustrated in Figures 3-9 and 3-10.



Level : RH70 (m)
Modelarea : (1545,6362)(1557,6374) RAK (km)
BP : Before Present

Figure 3-9. *Illustration of the shore displacement in the Simpevarp area since last glaciation /Rhén et al, 1997c/.*



Level : RH70 (m)
Modelarea : (1545,6362)(1557,6374) RAK (km)
BP : Before Present

Figure 3-10. *Illustration of the shore displacement in the Simpevarp area since last glaciation /Rhén et al, 1997c/.*

4 Description of Primary data for hydrogeological analysis

The primary data is mainly from field investigations and monitoring. In this chapter a brief overview of the hydrogeological investigations is reported. As pointed out in Chapter 1 this Site Investigation is performed in several steps increasing the amount of site-specific data for each step for the updating of the models.

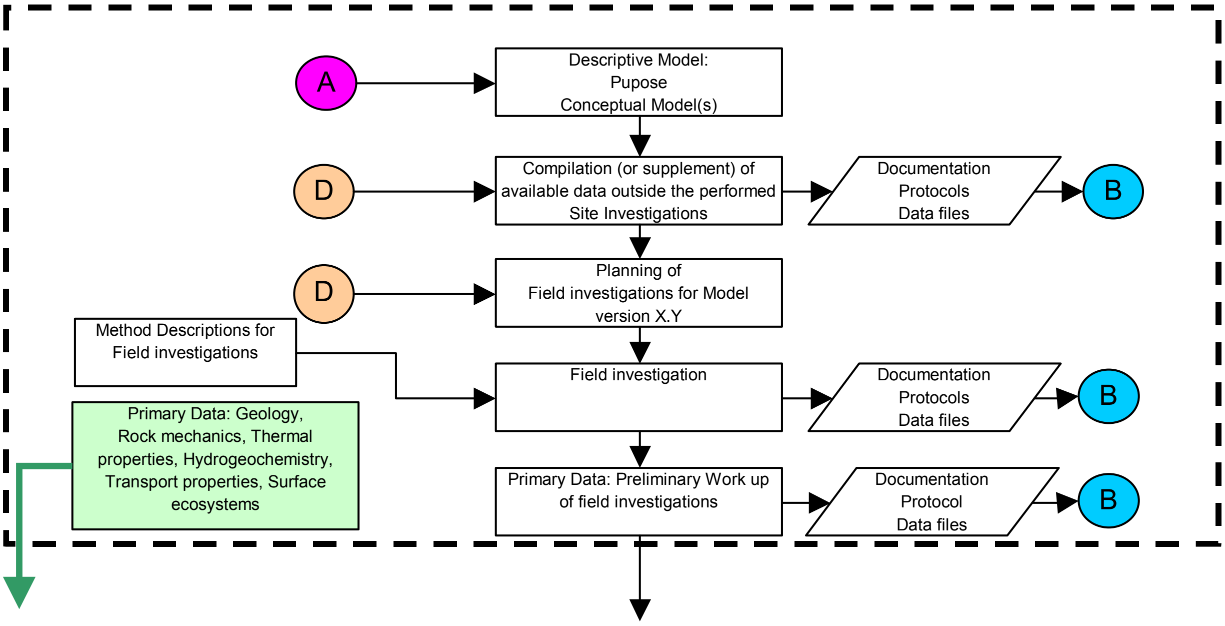


Figure 4-1. *An overview of the general performance of Site Descriptive Hydrogeological Modelling and the interaction with other disciplines. Part of flow chart shown in Figure 1-2 covering the Site Investigations. A, B, C and D show connections in the flow chart in Figure 1-2. A: Conceptual issues call for updating conceptual models. B: Data delivered or data received. C: Descriptive models are up dated because of the interactive and integrated modelling. D: New investigations needed to make the Descriptive models more detailed.*

4.1 Compilation of data other than Site Investigation data

To a large extent available data have been compiled in the 0 version model of the areas /Forsmark version 0, 2002; Simpevarp version 0, 2002/. In these reports data from other investigations (mainly from the power plants at Forsmark and Simpevarp and the CLAB facility in Simpevarp) were found. The usefulness of these data will be evaluated, and data deemed to be relevant will be compiled at an early stage of the Site Investigation in such a way that they can be used effectively in the ongoing Investigation. More data may be compiled at a later stage if considered to contain valuable information.

An inventory of private wells has been made previously, but may be complemented. A Method description, see Appendix 1, will serve as a guideline for a new inventory of borehole and construction data for hydrogeological documentation.

Meteorological, hydrological and oceanographical information up to the year 2001 has been compiled for sites under investigation /Larsson-McCann, 2002,a,b/. The time period differs between the data but several types of data have long time records. Most of the compiled data will be updated by SMHI (Swedish Meteorological and Hydrological Institute) ongoing measurements.

4.2 Field investigation planning

The 0 version model and /SKB, 2001b/ have been the base for the initial planning of field investigations. There will be more or less continuous planning in the course of Site Investigations. However, after each version of the descriptive model, the model will be scrutinized to see if the description fulfils Design and Safety Analysis requirements as well as those for a general understanding of the site. If not, new investigations will be performed. Suggestions pertaining to the type and location of investigations will be made.

4.3 Field investigations and Primary data

4.3.1 General description of planned hydraulic tests

Three types of test methods will be employed; constant-rate tests (pumping tests, flow logging), constant-pressure tests (injection tests) and variable head and flow rate tests (Slug tests). Several test method measurement sections are correlated to facilitate correlation studies between parameters.

Measurement scales (Test-section length, length of tested section in the borehole) generally will be used in bedrock are: Entire borehole, 100 m, 20 m and 5 m. Other test-section lengths may be chosen if for example a specific HCD is to be tested.

During pumping tests the temperature and EC of the out-flowing water are measured at the surface.

Several methods will be used to analyse the tests. In pumping and injection tests, the specific capacity (Q/s) and transmissivity are always calculated for the test section (flowing section) assuming stationary conditions in accordance with /Moye, 1967/. The interpretation method for transient tests (measurement of flow rate and pressure response as function of time) depends on the test method and interpretation of the flow regime of the measured response. The main interpretation methods considered relevant are described in /Horne, 1995/ and /Kruseman and de Ridder, 1990/.

Concerning slug tests, the most appropriate initial interpretation method is Cooper's method /Cooper et al, 1967; Papadopoulos et al, 1973/. Most interpretation methods for transient tests are based on the identification of time periods with 1, 2 or 3 dimensional flow fields, which form the basis for the interpretation of the hydraulic properties. This is also the case in all analyses of transient tests. All pumping and injection tests (and slug tests if test conditions are appropriate) are performed with two test phases; a flowing phase and a recovery phase. Both test phases are analysed separately and a set of parameters is chosen to represent the entire test and the evaluation period for the transmissivity (or hydraulic conductivity).

While interpretation methods based on fractional flow /Barker, 1988/ may be possible, they should not be used as a standard method for all tests.

Several types of hydraulic tests methods are planned. Common to all of them are the registering of measurement limits and representative water temperature and TDS values. Temperature and TDS cannot always be reported in conjunction with the reports on the field test but reasonable estimates for the transformation of the hydraulic properties to fluid-independent parameters can usually be made at later stages based on geophysical logging and/or water sampling.

Length calibration should normally be a part of all measurements made in core holes. The reason for this is that correlation studies of measured entities in long (deep) boreholes may not be possible unless length calibration is performed, as the tension in the cables/pipes holding the equipment may be several metres in a 1000 m deep borehole. Length calibration instructions, see Appendix 1 (MD 225.004), together with other method-specific MDs guide the length correction performance.

4.3.2 Hydrology

A new topographic map will be made based on aerial photography. This map, showing the location of watercourses, lakes and the coast as well, as the field inspection will serve as the base for defining surface water-divides. Field mapping of hydrology also includes documenting the positions of springs and probable discharge areas.

Runoff will be measured in a few watercourses. In some watercourses, continuous flow measurements will be made. These measurements will start in the initial Site Investigation phase.

Continuous water level measurements will be made in some of the lakes and in the sea.

One or possibly two meteorological stations will be established at each site. Measurements will include air temperature, precipitation, wind speed, air humidity and global radiation. Potential evapotranspiration will be calculated based on the measured variables.

Water samples will be taken from the sea in order to obtain TDS. Water sampling in lakes, watercourses and the sea is described in detail in /Löfgren and Lindborg, 2003/ and /Smellie et al, 2003/.

Method descriptions guide the establishment of new meteorological measurements, surface hydrological measurements and oceanographic measurements (MD 364.007, MD 364.008, MD 364.009, see Appendix 1).

4.3.3 Hydraulic properties of soil deposits based on geological documentation

The geological mapping of the soil deposits will be made by means of surface field mapping, the digging of pits, drilling, refraction seismics and airborn geophysics. The geophysics is expected to indicate the depth of the soil (regolith) with support of drillings. Soil samples will be taken during drilling and from the pits in what is deemed to be representative units, see /Munier et al, 2003/ and Appendix 1 (MD 131.001). Each sample will be visually classified and laboratory analysis will be made for selected samples in order to obtain grain-size distribution curves. The grain size distribution curve characteristics (d_{10}, d_{60}) are of particular interest (see Section 5.3).

4.3.4 Single-hole hydraulic tests – soil deposits

Pumping tests or slug tests will be performed in wells with screen in the soil deposits. These will be evaluated and reported in accordance with the slug test Method Description and Instruction for analysis of injection- and single-hole pumping tests (MD 325.001, MD 320.004, see Appendix 1). Transmissivity (T) and representative thickness for the Hydraulic conductivity (K) estimate of the geological unit is interpreted from the test. A representative measurement of water temperature and TDS is also reported. Evaluation of a pumping test may also provide the skin factor for the well, leakage conditions and indications of other boundary conditions.

4.3.5 Interference tests – soil deposits. Preliminary evaluation

"Preliminary evaluation" refers to the evaluation of all geometric and geological data that are unlikely to be available after the tests have been performed. However, some preliminary interpretations can probably be made at the same time as the report on the field test. The conditions for interpreting an interference test are best during the analysis of Primary data and during the integrated modelling phase, see Chapters 5 and 6.

A possible reason for Interference tests in the surficial deposits may be to evaluate the properties and geometry (if possible) of some more permeable geological unit. The Transmissivity (T) and representative thickness for the Hydraulic conductivity (K) estimate of the geological unit is interpreted from the test. Representative water temperature and TDS are also reported as well as preliminary assessments of boundaries, leakage conditions and the skin factor for the well.

These tests will be evaluated and reported according to the interference test Method Description and Instructions for the analysis of injection- and single-hole pumping tests (MD 303.003, MD 320.004, see Appendix 1). The interference tests will be partly re-analysed when the three-dimensional modelling starts (Chapter 6), based on the defined geological domains of the surficial deposits. The results from the interference test may influence the assessment of the extent of the domain.

4.3.6 Drilling of boreholes in rock and measurements during drilling

During drilling several parameters are measured as described in several Method Descriptions: Percussion drilling, Method description for core drilling, Method description for registration of drilling parameters and sampling of drilling water as well as drill-cuttings during core drilling (MD 610.003, MD 620.003, MD 640.001, see Appendix 1). The main purpose is to obtain information leading to an overview of the rock and hydraulic conditions to facilitate water sampling decisions during drilling. It also serves the purpose of facilitating balance calculation for the borehole related to drilling fluid and drill-cuttings.

The tests in 100 m test scale are performed during the drilling of the core hole or sometimes after drilling has been completed. During the drilling of a core hole, the natural (undisturbed) pressure of the last drilled part of the borehole, approximately 30–50 m, is usually measured over a 6–12 h period. Pump test Method description, pressure measurement and water sampling in connection with wireline drilling (MD 321.002, see Appendix 1) serve as a guideline for the tests and the sampling during drilling.

4.3.7 Flow logging CF – rock mass

Flow logging takes place in percussion drilled and core boreholes by means of an impeller technique. The purpose is to define the cumulative flow distribution along the borehole during pumping. The flow rate distribution and the evaluated transmissivity for the entire borehole are used to estimate the transmissivities of the flow anomalies. The cumulative T-distribution is calculated as follows:

$$\sum T_i = T \cdot \frac{\sum Q_i}{Q_p}$$

Where Q_p is the pump rate measured at the surface, ΣQ_i is the corrected logging flow rate (the flow rate distribution during pumping minus the natural flow distribution without pumping. Natural flow distribution may generally be below the measurement limit with methods used.) and transmissivity (T) representative of the entire hole. T is generally estimated from the draw down or recovery phase of the pumping period before or after the flow logging. The execution of the flow logging is based on Method description MD 322.009 (see Appendix 1).

The measurement range is different compared to Flow logging with PFL. The lower as well as the upper measurement limits are higher for CF than PFL. The main purpose of logging in the core hole is therefore to be able to measure high transmissive features, which may be above the PFL measurement limit. CF in core holes is not performed if PFL measurements have provided sufficiently good data.

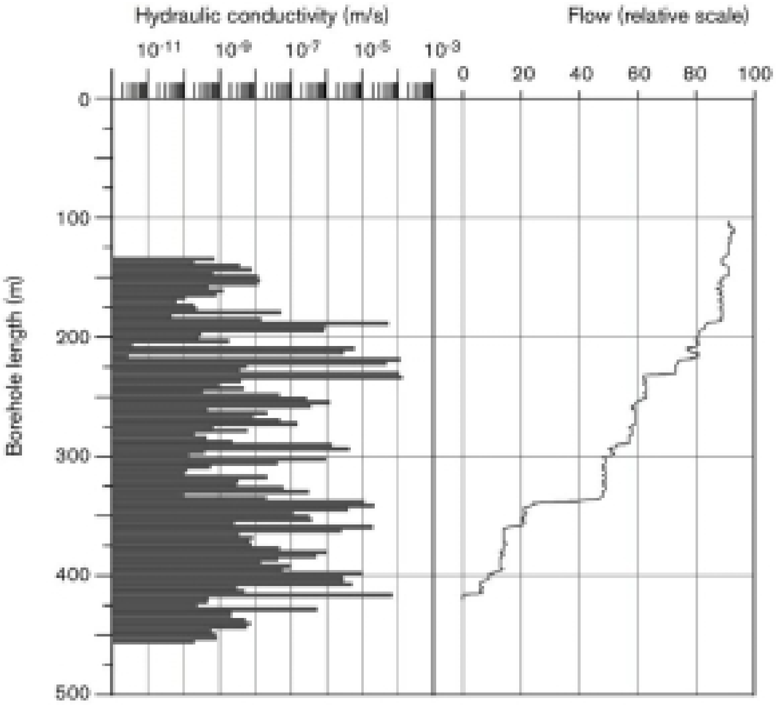


Figure 4-2. *Example of results from flow logging with CF and injection tests.*

4.3.8 Flow logging PFL – rock mass

The Posiva Flow Log (PFL) can only be used in core holes. The selected method is called Difference Flow Meter (DIFF) and is illustrated in Figures 4-3 and 4-4. The method can be operated in several modes, and the preliminary modes that will be used are shown in Table 4-1. The measurement section length (L) is limited by rubber discs, and the distance the measurement section is moved is called step length (dL). The measurement section is either moved dL=L after each test (Sequential flow logging) or with a dL<L (Overlapping flow logging). The benefit of Overlapping flow logging is that it is possible to fairly accurately identify flow anomalies along the borehole. The flow anomalies are mostly connected to a fracture or fracture zone in the core mapping.

If two different drawdowns are used for two flow logging sequences, the approximate transmissivity and the approximate undisturbed pressure can be calculated, based on the theory for radial, stationary flow with an assumed radius of influence. Details of the performance of the flow logging can be found in MD 322.010 (see Appendix 1).

The natural flow in or out of the measurement section (Q_0) and the estimated undisturbed pressure in the measurement section (p_0) are useful for water budget considerations from a hydrogeochemical point of view under open borehole conditions. EC and absolute pressure at measurement section level (p_t) are important for the overall evaluation of each measurement section result. Temperature and EC are useful for estimating fluid independent parameters.

The transmissivity of the flow anomalies may be estimated by combining the results from sequential and overlapping flow logging. For example, the transmissivity of a flow anomaly (T_n), located within a longer section, e.g. 5 m, can be estimated from the calculated

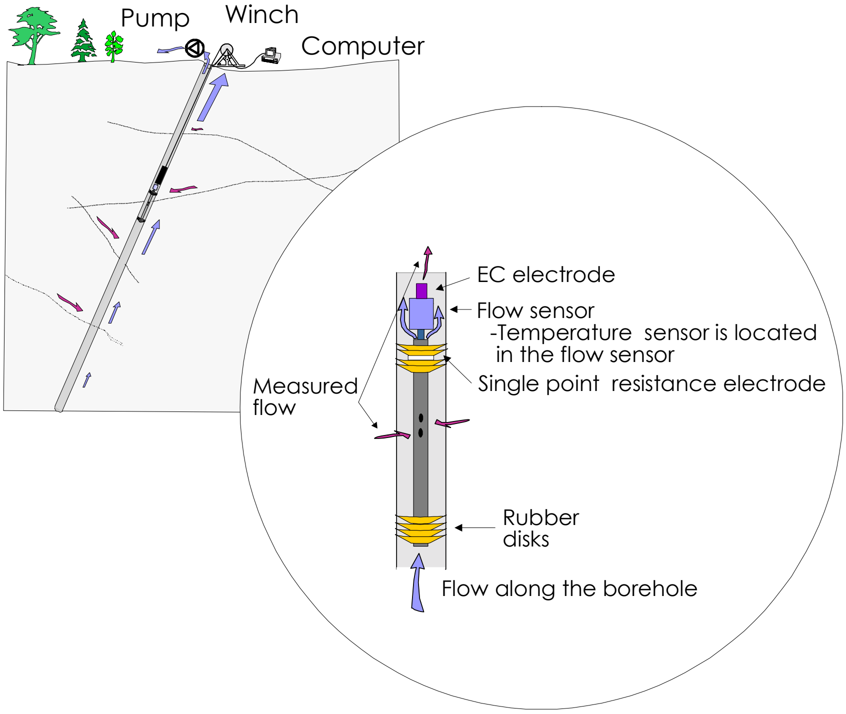


Figure 4-3. *Detail of the down-hole tool in difference flow logging (DIFF).*

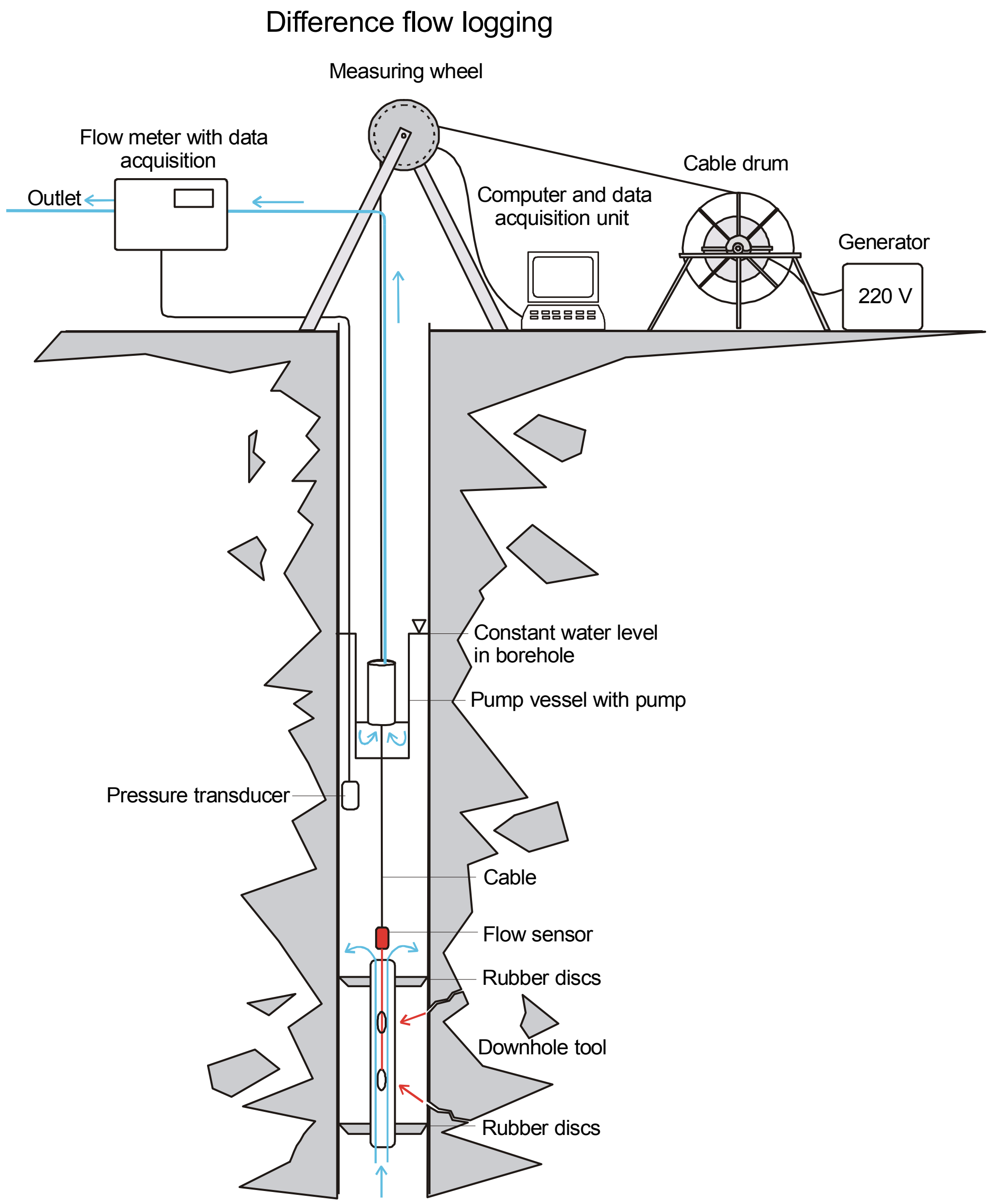


***Figure 4-4.** Schematic of the equipment used in difference flow logging (DIFF).*

transmissivity of the longer section (T_5) from the sequential logging and the sum of the measured flows ($\Sigma_5 Q_n$) in the longer section (5 m) during the overlapping flow logging in shorter sections, according to the following equation:

$T_n = T_5 \cdot Q_n / \Sigma_5 Q_n$

Flow anomalies (and Single Point Resistance, SPR) can then be compared to the core mapping to identify specific fractures or fracture zones. Fractures with a transmissivity larger than the measurement limit can then be coupled to core mapping data such as fracture orientation. The data can thus be used to estimate the anisotropy.

Further details about PFL can be found in /Öhberg and Rouhiainen, 2000/.

Table 4-1. Preliminary Difference flow logging programme for SKB Site Investigations. (EC: Electrical Conductivity, SPR: Single Point Resistance. Te: temperature, Q_0: Natural flow in or out of the measurement section, open hole conditions and no pumping, Q_x: Flow from measurement section during pumping, p_t: Absolute pressure at measurement section level.)

Measurement program	Measurement mode	Head difference applied (kPa)	Measurement section length (L) (m)	Step length (dL) (m)	Measured entities	Comments
Initial measurements						
	Length calibration	0	One rubber disc		Caliper and SPR	
	Measurement of the borehole fluid	0	One rubber disc!		EC and Te	
Standard programme						
	Sequential flow logging	0	5	5	Q_0 P_t EC SPR	
	Sequential flow logging	100	5	5	Q_x P_t EC SPR	
	Overlapping flow logging	100	1	0.1	Q_x P_t EC SPR	Base for Conductive fracture frequency estimate
Hydrogeochemistry programme						
	Overlapping flow logging	100	5	0.5	Q_x P_t EC SPR	
	Sequential flow logging	0	5	5	Q_0 P_t EC SPR	
	Overlapping flow logging	100	1	0.1	Q_x P_t EC SPR	Base for Conductive fracture frequency estimate
Optional programme						
	Fracture EC measurements	100	1	0.1	Q_x P_t EC SPR	Long duration of pumping to obtain EC for a fracture

4.3.9 Single-hole transient hydraulic tests – rock mass

Pumping tests will be performed in open boreholes or packed-off test sections in percussion drilled and core holes. Either the entire borehole is pumped or a section is packed-off. The tests are performed as constant-rate tests (pumping tests) or constant-pressure tests (injection tests).

Generally the pumping test starts with a short capacity test to obtain data for selecting a suitable flow rate for the test. After the capacity test, the pressures are left to recover during a period of time, while the natural conditions are measured to gauge any trends in the formation. In Table 4-2 the recommended test phase duration is shown.

The fieldwork is guided by the Method description for hydraulic single-hole pumping tests (MD 321.003, see Appendix 1). The tests will be evaluated and reported in accordance with the Instructions for the analysis of injection- and single-hole pumping tests (Appendix 1, MD 320.004) while the pump test pressure measurement and water sampling will be evaluated in connection with wireline drilling (Appendix 1, MD 321.002). Transmissivity (T) and representative thickness for the T estimate of the geological unit is interpreted from the test. Representative water temperature and TDS are also reported. The evaluation of a pumping test may also give the skin factor for the well, leakage conditions and indications of other boundary conditions.

Table 4-2. Recommended test phase durations.

Test type	Test section length (m)	Test type	Capacity test	Stabilisation	Flow period	Recovery period	Comment
Injection test	5	Constant pressure: 200 kPa	No	15 min	15 min	15 min	
Injection test	20	Constant pressure: 200 kPa	No	30 min	30 min	30 min	
Pumping test	5–100	Constant rate	Yes	3 h	3 h	3 h	Duration depends on the purpose of the test
Pumping test	Entire borehole	Constant rate	Yes	Ca 1 day	1–2 days	0.5–1 day	Duration depends on the purpose of the test

4.3.10 Interference tests – rock mass. Preliminary evaluation

"Preliminary evaluation"; see Section 4.3.5.

High-quality interference tests

Interference tests with a pumping section in a borehole drilled in rock and response measurements in observation boreholes are carried out to evaluate the properties and (if possible) some geometrical property of the rock mass. Either the entire borehole or a packed-off section is pumped. The tests are performed as constant-rate tests.

Generally the measurements start with a short capacity test to obtain data for the selection of a suitable flow rate for the test. After the capacity test the pressures are let to recover for 2–3 days while the natural conditions are measured to gauge any trends in the formation. The pumping period is generally 3 days followed by a recovery period of 1–2 days. A few Long-term Pumping Tests (LPT) will be performed, with pumping and recovery periods of 3–6 months and 1–2 months respectively. A tracer test may be carried out in conjunction with the LPT (then called Long-term Pumping and Tracer Test (LPTT). In some of the pumping tests, dilution tests will be performed in selected borehole sections.

Transmissivity (T), and if possible storage coefficient (S), of the pumped HCD or the T for the entire borehole are interpreted from the test. A representative water temperature and TDS is also reported as well as preliminary assessments on the connectivity between HCDs, boundary conditions, leakage conditions and the well skin factor. Data from the tests are also essential for the calibration of groundwater flow models.

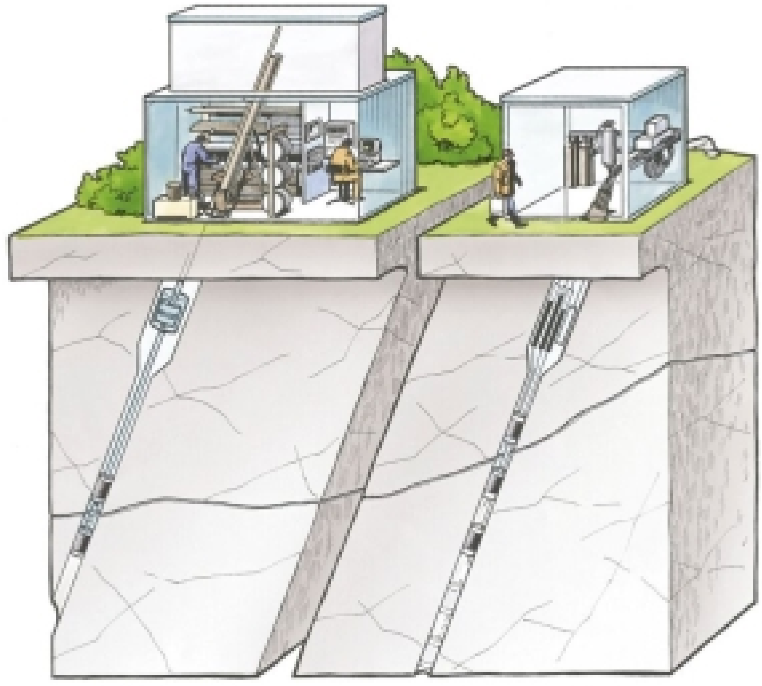


Figure 4-5. *Interference tests with multi-packer system in observation boreholes.*

These tests will be evaluated and reported on in accordance with the interference test Method Description and Instructions for analysis of injection- and single-hole pumping tests (see Appendix 1, MD 303.003, MD 320.004). The interference tests will be partly re-analysed when the three-dimensional modelling starts (Chapter 6), based on the geological domains defined for the deterministic deformation zones and rock domains. The results from the interference test may influence the assessment of the positions and extent of the deterministic deformation zones and rock domains.

Low-ambition interference tests

If observation boreholes are available within 500–1000 m from a borehole that is being drilled or hydraulically tested, it can be practical to carry out continuous monitoring of the observation boreholes. Pressure responses may be difficult to interpret quantitatively but can provide useful information on hydraulic connectivity that may indicate the presence of significant hydraulic features and large-scale anisotropy. These interference tests will also be partly re-analysed when the three-dimensional modelling starts (Chapter 6), based on the geological domains defined for the deterministic deformation zones and rock domains.

4.3.11 Dilution tests

The groundwater flow in a saturated geological formation can be estimated from dilution measurements, see for example /Halevy et al, 1967; Drost et al, 1968; Gaspar and Oncecu, 1972/. The tests are generally performed using a permanently installed packer system in the boreholes, see Figure 4-6 but may also be made with a SKB developed probe /Gustafsson, 2002a,b/. The dilution rate is either measured in natural conditions or during a pumping test of long duration. Dilution tests are described in more detail in /Berglund and Selroos, 2003/.

4.3.12 Long term monitoring of piezometric levels

After all tests have been performed in a borehole, a packer system is usually installed, see Figure 4-6. Observation boreholes in soil deposits consist of a pipe with one screened part, and no packers are therefore installed in those pipes.

Piezometric levels are measured with a data logger. Manual logging of the water levels in the standpipes or open borehole takes place for calibration purposes. Water in the standpipes is pumped in order to obtain the same fluid density in the standpipes as in the observation section. The electrical conductivity of the pumped water is measured to estimate the fluid density.

When the measurement system is installed, the natural variation in piezometric levels as well as responses during interference tests can be measured.

Performance test should be performed of observation boreholes in soil deposits to judge their hydraulic connection to the formation.

The number of borehole sections in rock is dependent on the length of the borehole and number of interpreted significant hydraulic conductors. The open borehole between packed off sections is a significant conductor that short-circuit intersecting fractures, it is therefore preferable to have not too long observation sections but it is also limitations of the number of sections that can be installed. The maximum number of section that can be installed depends on the diameter of the borehole and the number of sections for dilution measurements. In a borehole with diameter 76 mm the maximum measurement sections that can be installed is 10 sections for pressure with two of them being sections for dilution measurements. In percussion boreholes the maximum measurement sections that can be installed is 4 sections for pressure with one of them being section for dilution measurements.

For dilution measurements a short measurement section is preferred to minimize the water volume in the section. Installing a dummy in the measurement section can decrease the water volume

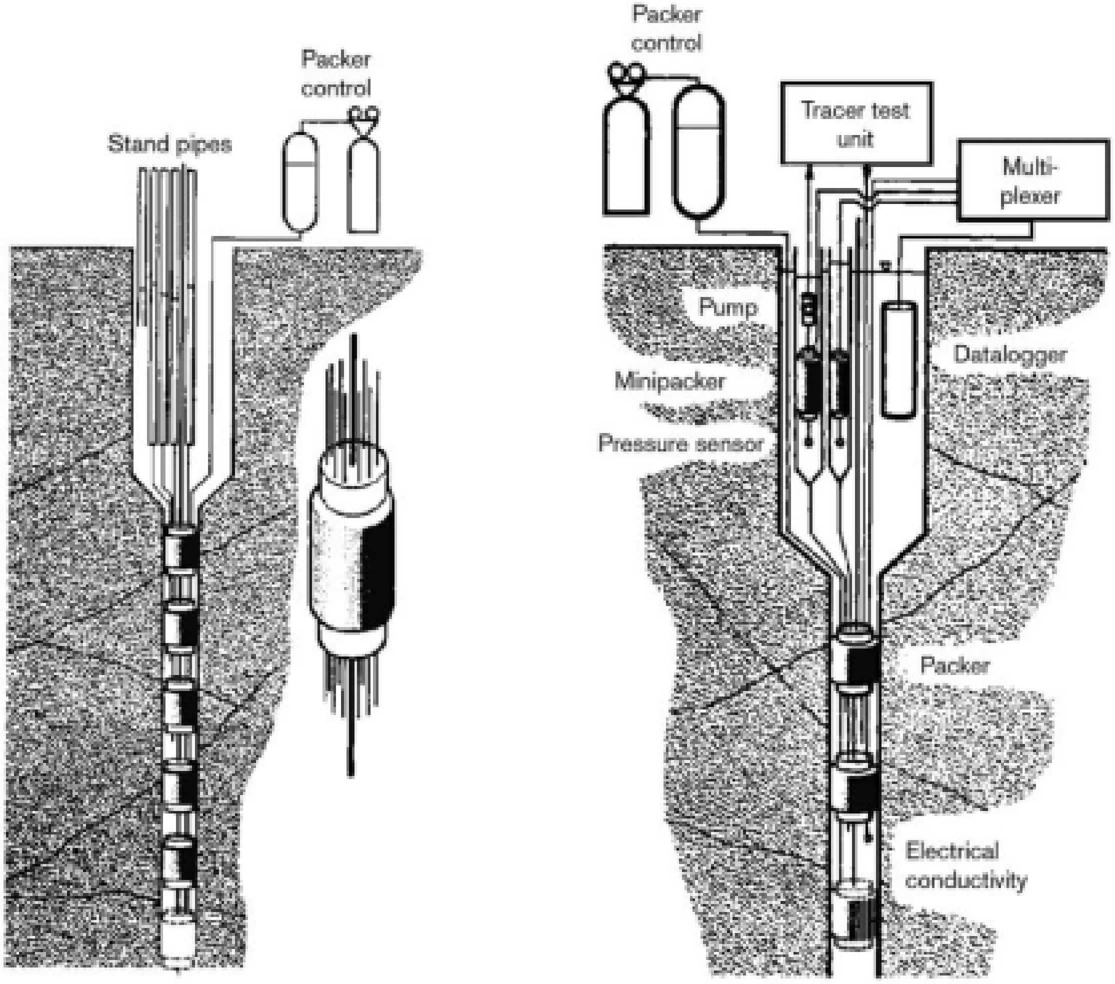


Figure 4-6. *Illustration of the monitoring system for pressure measurements and dilution tests.*

5 Hydrogeological analysis of primary data

The hydrogeological analysis of primary data presented in this chapter is made for the purpose of compiling, categorising and making an initial evaluation of the data, without the input of other disciplines. The work consists of compiling monitoring data (precipitation, run-off data, piezometric levels etc) and making some initial compilation and analysis of data from hydraulic tests. If the results of investigations of rock segments /see Munier et al, 2003/ along the borehole are available, they will be included in this analysis. The purpose is to obtain an overview and compilation that facilitates the effective communication of three-dimension modelling as outlined in Chapter 6. Figure 5-1 illustrates the work.

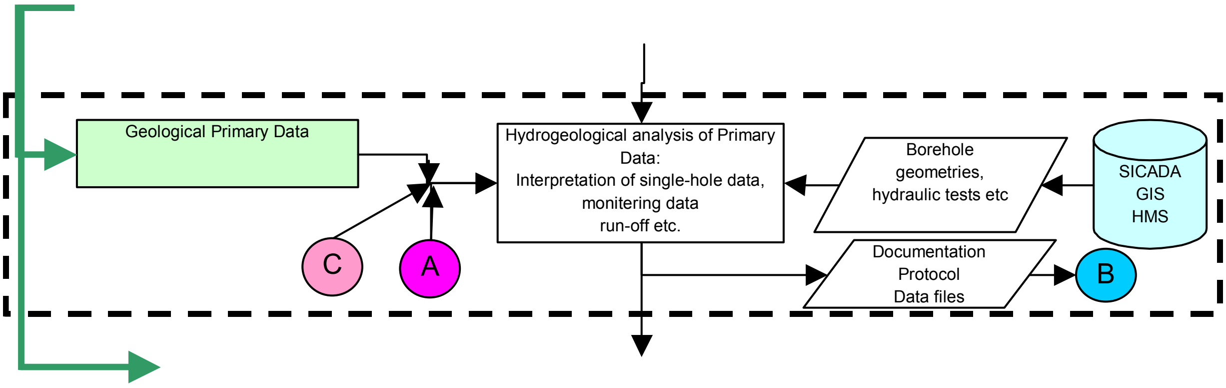


Figure 5-1. *An overview of the general performance of Site Descriptive Hydrogeological Modelling and the interaction with other disciplines. Part of flow chart shown in Figure 1-2 covering the Hydrogeological analysis of primary data. A, B, C and D show connections in the flow chart in Figure 1-2. A: Conceptual issues call for updating conceptual models. B: Data delivered or data received. C: Descriptive models are up dated because of the interactive and integrated modelling. D: New investigations needed to make the Descriptive models more detailed.*

5.1 General analysis of primary data

5.1.1 Quality Control of primary data

The reports on the hydraulic test results stored in the database are checked. All tests results are also plotted and analysed in order to identify any outliers that require further checking to ensure that the data has been correctly reported and that the interpretation seem reasonable. The conventional Box-and-Whisker plot of the actual values or of the Log_{10}(measured value) is one tool used for the screening.

If some data appear to be erroneous, the responsible activity leader is contacted to discuss how to resolve the issue. The person responsible for the performance of the task and the delivered data will probably also need to be contacted.

5.1.2 Water properties

In cases where it has not proved possible to report TDS and temperature in conjunction with the delivery of the hydraulic test results, the database is updated with other measurements. The source of information is primary water samples from test section with EC or TDS that can be considered representative as well as temperature measurements from borehole logging. Water temperature measurements may be lacking for boreholes in areas of surficial deposits, but an approximate estimate of water temperature can be made from a depth below the ground surface during the months in which the hydraulic test is performed.

For a test section comprising only EC, the TDS-value is calculated according to the equation below /Rhén et al, 1997c/. This equation may be updated in line with new site data, after which it can be included in the hydrogeochemical description.

$$TDS = \frac{0.00467}{0.741} \cdot EC$$

EC: Electrical conductivity of water (mS/m)

TDS: (g/L)

The density and dynamic viscosity of the water is then calculated in accordance with /e.g. Horne, 1995/, based on the temperature and TDS, assuming that NaCl in the equations can be approximately represented by TDS. The Fluid Coefficient for the intrinsic permeability (FC_T) and porosity-compressibility-product (FC_S) are then calculated, as presented in Chapter 3, and the influence of temperature and TDS on the hydraulic parameters is assessed.

5.1.3 Overview of primary data – WellCad

Selected core mapping parameters and percussion drilling and geophysical logging documentation are plotted together with different types of results from hydraulic tests in order to obtain an overview of the primary data. An example of a standard plot used in a project at Äspö HRL is shown in Figure 5-2. New standard plots will be made for core and percussion holes.

The core mapping is the base for a preliminary division of the interpreted hydraulic properties (mainly hydraulic conductivity) into possible geological units and subsequently HCDs and HRDs.

5.1.4 Analysis of primary data

Hydraulic test results, natural fractures, crush and rock types are the basis for the analysis of the rock mass. The available geological mapping of each borehole in the soil as well as the existing geological description of the soil of the site are of primary importance for the initial interpretation of the hydraulic properties of the soil.

Some preliminary correlation studies are performed and statistics produced from the available material. First description statistics are mainly univariate.

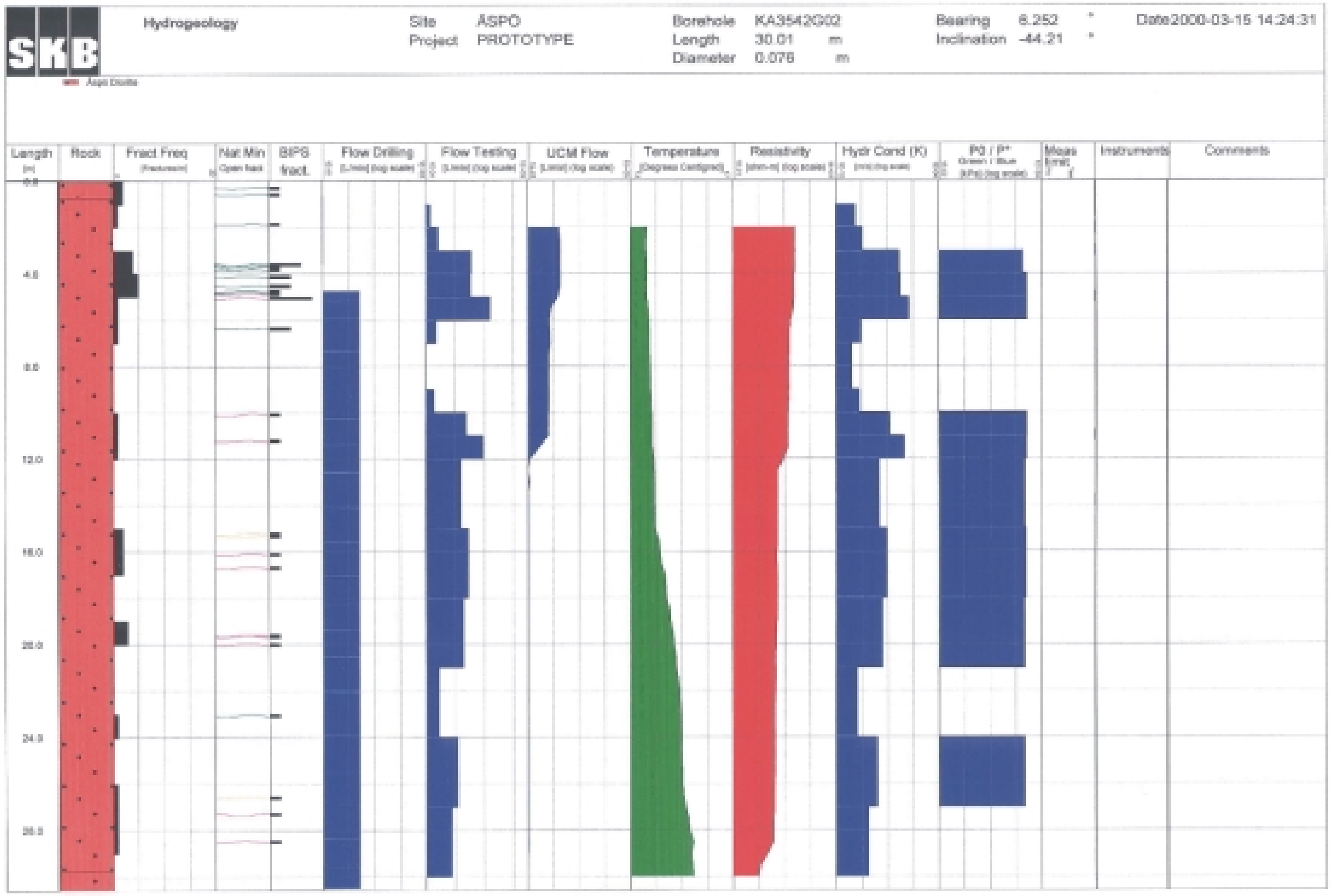


Figure 5-2. *Data overview of core holes. Example of overview of selected core mapping data and results from hydraulic tests illustrated by means of WellCad.*

5.1.5 Statistical analysis

Univariate statistics are used to obtain an overview of measurements of different kinds. An example based on borehole data is provided below.

For each measurement scale, univariate statistics are used to evaluate the systematic measurements along the boreholes. Indications of conductive features with higher permeabilities than the surrounding rock or geological interpretations of intersecting deformation zones and rock-segments /see Munier et al, 2003/ along the borehole are used to group the data set into borehole sections representing possible HCDs and HRDs. Mapped rock types along the borehole are also used to group the data into sub-sets for statistical analysis. Figures 5-3 to 5-4 illustrate the estimation of the statistical distribution of a data set. In the analysis, upper and lower measurement limits are taken into account.

The general assumption is that transmissivity or hydraulic conductivity is lognormal-distributed and therefore only transformed data are analysed; Log$_{10}$(T), Log$_{10}$(K). The arithmetic mean and standard deviation of the transformed distribution are reported, and the data agreement with the probability distribution function (pdf) or cumulitive distribution function (cpf) is also noted. Other distributions may be tested if required.

A geostatistical analysis is also made of the borehole data. The borehole data are however only used to study the correlation with the semivariogram analysis along the boreholes. The purpose of this is to evaluate correlation models in terms of whether or not the patterns can indicate correlation structure and periodicity /Isaaks and Srivastava, 1989; Deutsch and Journel, 1997; Jensen et al, 2000; Deutsch, 2002/.

Observations of the bedrock surface will be based on drilling through the soil deposits and on mapped outcrops, refraction seismic, airborne geophysics and mapped bedrock surfaces from previous investigations. These data will be used to estimate a semivariogram for the bedrock surface and for modelling the bedrock surface.

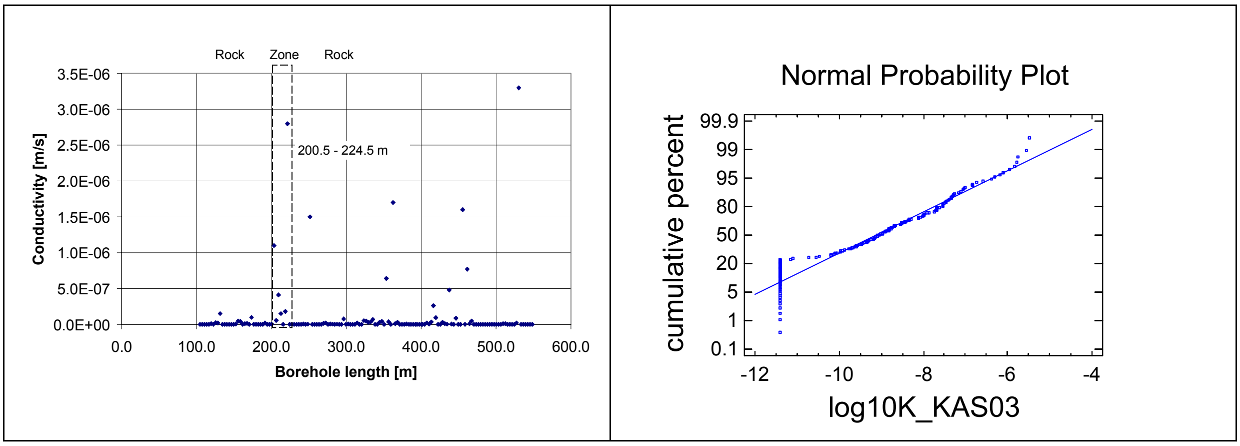


Figure 5-3. *Left: Example of the distribution of K along a borehole, preliminary evaluation of the position of HCD. Right: Cumulative probability distribution of Log*$_{10}$*K for the entire data set for the borehole. Estimated Log*$_{10}$*K lower and upper measurement limits are –10.20 and –5.79 (K in m/s).*

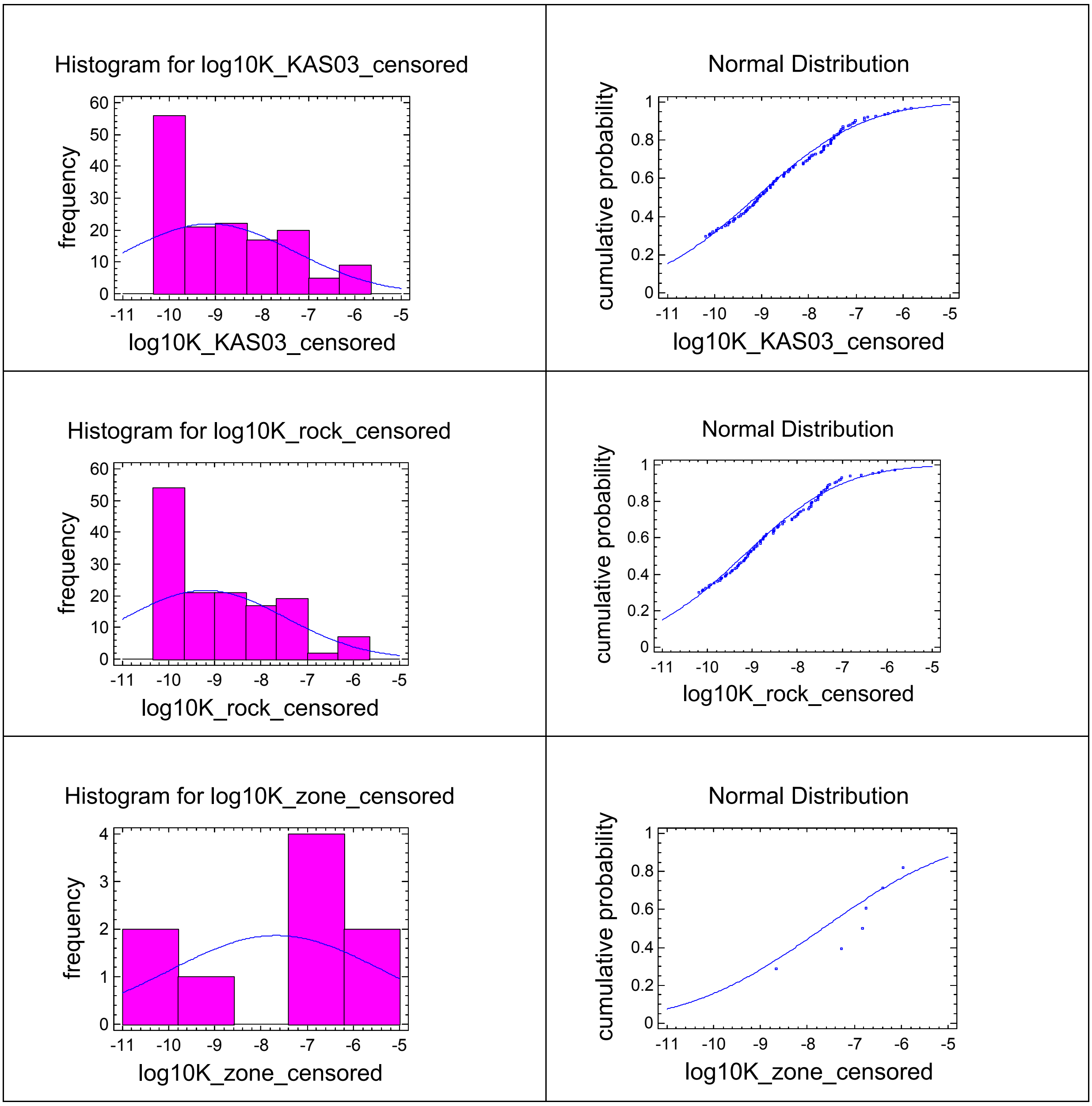


Figure 5-4. *Example on the distribution of Log$_{10}$K for a borehole. Top: Entire borehole, Middle: Suggested HRD. Bottom: Suggested HCD. Estimated Log$_{10}$K lower and upper measurement limits –10.20 and –5.79 (K in m/s) have been considered in the analysis. Measurement limit values are shown in the histograms but are not included in the cumulative probability plot (K in m/s).*

5.2 Hydrology

The location of watercourses, lakes and the seashore, topographic map as well as hydrology field mapping, provides data for defining surface water-divides and probable discharge areas, see Figures 5-5 to 5-7.

Characteristic runoff values are calculated based on the location of lakes and catchment areas (LLQ50, MLQ, MQ, MHQ, HHQ50)[1] /Vägverket, 1990/. The continuous flow measurements of watercourses will also be compiled.

The continuous water level measurements in lakes and in the sea and from the SKB operated meteorological stations will be documented. Meteorological, hydrological and oceanographic data from nearby stations that are considered relevant are reported and stored in the database.

TDS of sea water sampling is of special hydrogeological interest and will be documented. TDS is described in more detail in /Löfgren and Lindborg, 2003/ and /Smellie et al, 2003/.

Monitoring data from boreholes are documented in order to obtain an overview of the variation over time and the influences of performed hydraulic tests.

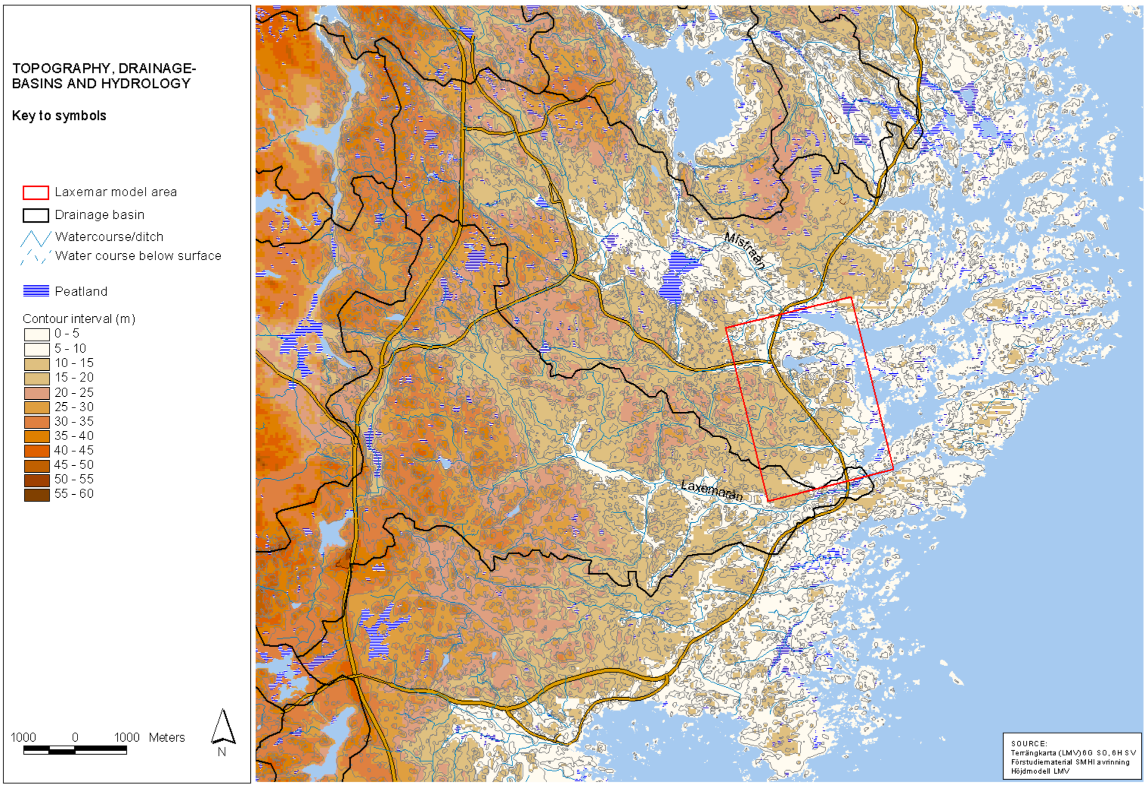


Figure 5-5. Surface water divide (Drainage basin), watercourses and topography in and near the Laxemar area /Andersson et al, 2002a/.

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[1] LLQ50: Lowest minimum runoff 50 year recurrence interval, MLQ: Long-term minimum average runoff, MQ: Long-term average runoff, MHQ: Long-term maximum average runoff, HHQ50: Long-term maximum runoff 50 year recurrence interval.

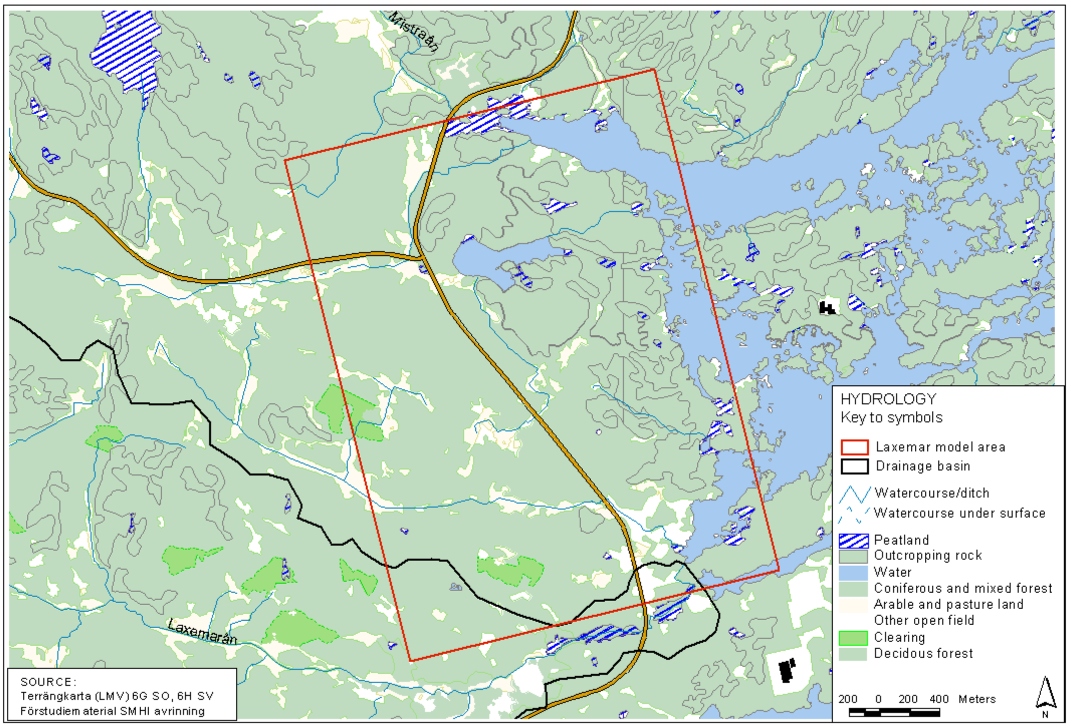


Figure 5-6. *Surface water divide (Drainage basin), watercourses and generalised vegetation description in and near the Laxemar area /Andersson et al, 2002a/.*

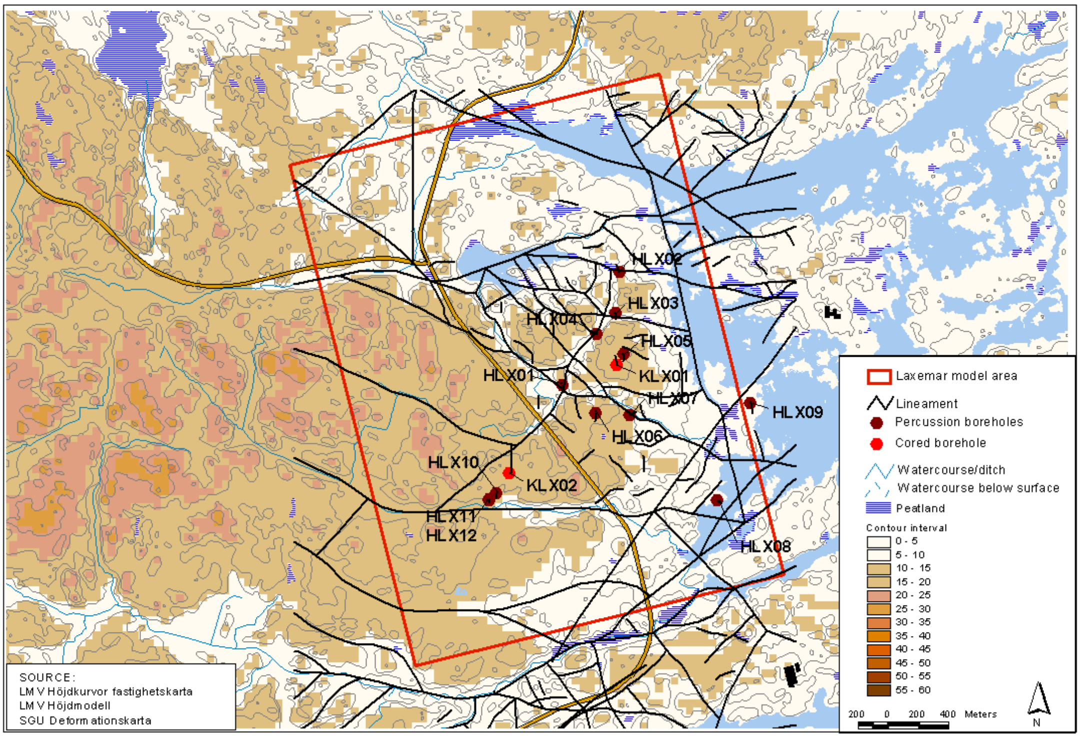


Figure 5-7. *Topography of rivers, lineaments and boreholes, watercourses in and near the Laxemar area /Andersson et al, 2002a/.*

5.3 Soil properties based on geological documentation

The grain size distribution curve characteristics (d_{10}, d_{60}) are used to estimate the hydraulic conductivity of the samples in accordance with /Gustafson, 1983/. The geological description of the samples forms the base for a preliminary division of the samples into possible geological units and ultimately HSDs.

5.4 Hydraulic tests

Hydraulic tests are reported in fairly great detail, and if transient tests have been performed a flow regime interpretation should be available. The plotting of pressure derivatives and comments concerning the flow regime are scrutinised to see whether the interpretation seems valid and agrees with the available data. Some complementary analysis may be conducted at this stage but generally some re-interpretation of interference tests takes place during the three-dimension modelling phase as outlined in Chapter 6.

5.4.1 Single-hole hydraulic tests – Soil deposits

The geological description of the samples taken during the installation of the observation boreholes is the base for a preliminary division of the interpreted hydraulic properties (mainly hydraulic conductivity) into possible geological units and ultimately HSDs. The available geological description of the soil deposits at the site is used. Of special interest are hydraulic tests indicating leakage and boundary conditions. These tests are scrutinised in the light of the available geological description in order to interpret geometric and leakage conditions for discussion with the geologists at a later stage.

5.4.2 Interference tests – Soil deposits

Responses in observation boreholes in surficial deposits and borehole sections at the top of the rock mass are interpreted by means of distance-drawdown plots, time-drawdown plots and response times (time lag, t_L) to achieve a pressure change of 1 kPa at observation sections after cessation of pumping. Distances to boundaries are calculated, if possible. The available geological description of the soil deposits at the site is used for the purpose of comparison with the hydraulic test interpretation. Of special interest are responses indicating leakage, boundary conditions and anisotropic conditions. These tests are scrutinised in the light of the available geological description in order to interpret geometric and leakage conditions for discussion with the geologists at a later stage.

5.4.3 Flowlogging CF – rock mass

The cumulative transmissivity along the borehole, interpreted flow anomalies, EC and temperature are plotted together with selected core mapping data. Of special interest are borehole sections indicating possible HCDs.

5.4.4 Flowlogging PFL – rock mass

Hydraulic parameters interpreted from hydraulic tests with measurement scales (L) and step lengths (dL); (L,dL): (1, 0.1), (5, 5) and (5, 0.5) and interpreted flow anomalies are plotted together with selected core mapping data (L and dL in meter). Of special interest are borehole sections indicating possible HCDs. Data are explored by means of univariate statistics.

The flow anomalies, with interpreted transmissivities, are compared with the core mapping in order to identify corresponding single fractures or fracture groups. These data containing a sub-set of the natural fractures with transmissivities are analysed as discussed in Chapter 6 so as to identify different fracture sets that may show anisotropic hydraulic conditions.

5.4.5 Single-hole transient hydraulic tests – rock mass

The core mapping is the basis for a preliminary division of the interpreted hydraulic properties (mainly hydraulic conductivity) into possible geological units and ultimately HCDs and HRDs. The available geological rock mass description is used.

Hydraulic parameters interpreted from hydraulic tests, the most common measurement scales of which are 5, 20, 100 m and entire boreholes, and flow logging data are plotted together with selected core mapping data. Of special interest are borehole sections indicating possible HCDs. Data are explored by means of univariate statistics.

Hydraulic tests of longer duration may indicate leakage and boundary conditions. These tests are scrutinised in the light of the available geological description in order to interpret geometric and leakage conditions for discussion with the geologists at a later stage.

5.4.6 Interference tests – rock mass

Responses in observation boreholes in soil deposits and borehole sections in the rock mass are interpreted with distance-drawdown plots, time-drawdown plots and response times (time lag, t_L) to achieve a pressure change of 1 kPa in the observation section after the cessation of pumping. Distances to boundaries are calculated where possible. The available geological description of the rock mass and the soil deposits of the site are used for the purpose of comparison with the interpretation. Of special interest are responses indicating leakage, boundary conditions and anisotropic conditions. These tests are scrutinised in the light of the available geological description in order to interpret geometric and leakage conditions for discussion with a geologist at a later stage.

5.4.7 Dilution tests

The flow rates through borehole sections in the course of natural (undisturbed conditions) and different interference tests, measured with dilution technique, are compiled to obtain an overview of the collected data. These data are used in the three-dimensional modelling to indicate the magnitude of natural flow rates in the rock mass (assuming a correction factor for the hydrodynamic field distortion by the borehole) and connectivities between HCDs.

6 Three-dimensional modelling and Site Description

Three-dimensional modelling is an integrated activity and involves the disciplines of Geology, Rock Mechanics, Thermal properties, Hydrogeology, Hydrogeochemistry, Transport Properties and Surface Ecosystem. The purpose is to obtain a consistent site description based on a defined set of available data. Three-dimensional modelling is intended to be carried out in steps in order to obtain an X.Y version model for the investigation phase in question. In cases necessitating the determination of HCD and HRD properties, the input from the discipline of Geology is most important, although certain aspects of Rock Mechanics and Hydrogeochemistry are important for the re-analysis of the data.

The hydrogeological analysis of primary data presented in Chapter 5 is performed more or less independently of the geologist's interpretation of the core mapping. The primary data analysis provides indications of whether or not HCDs are anomalies in the measured transmissivity distributions along the boreholes. Natural fracture frequency and crush are core mapping data that should to some extent correlate with to the interpreted transmissivity distributions. It can also be assumed that Rock type distributions may correlate with the transmissivity distributions. It is further tested the correlation between hydraulic parameters and *rock segments* along boreholes interpreted by geology. Interference tests may have confirmed connectivities between previously deterministically defined deformations zones or indicated possible new larger deformation zones. Large scale tracer and interference tests are useful for the integrated evaluation.

Groundwater flow simulations are an essential part of hydrogeological 3D modelling, as the descriptive model can be tested in several ways to determine how well it can replicate the observations made. The calibrated groundwater flow model forms a large part of what can be considered the Hydrogeological Site Descriptive Model. The forward simulations of flow paths and particle tracking are useful for several disciplines such as Hydrogeochemistry, Transport and Surface Ecosystem.

Groundwater flow modelling will provide flow paths from recharge areas to discharge areas. In combination with the geological description of the soil and the rock mass, these flow paths will be essential for the hydrogeochemical understanding and interpretation of the measured water compositions.

Rock mechanics stress modelling indicates stress magnitudes and stress ratios, which in turn may indicate the major directions of hydraulic anisotropy. Hydraulic data in combination with the stress model may lead to an enhanced understanding of the influence of stress on the hydraulic properties of the rock mass.

This chapter is intended to describe the 3D modelling with the interaction with other disciplines and the iterative approach to update the hydrogeological models. Figure 6-1 illustrates the work.

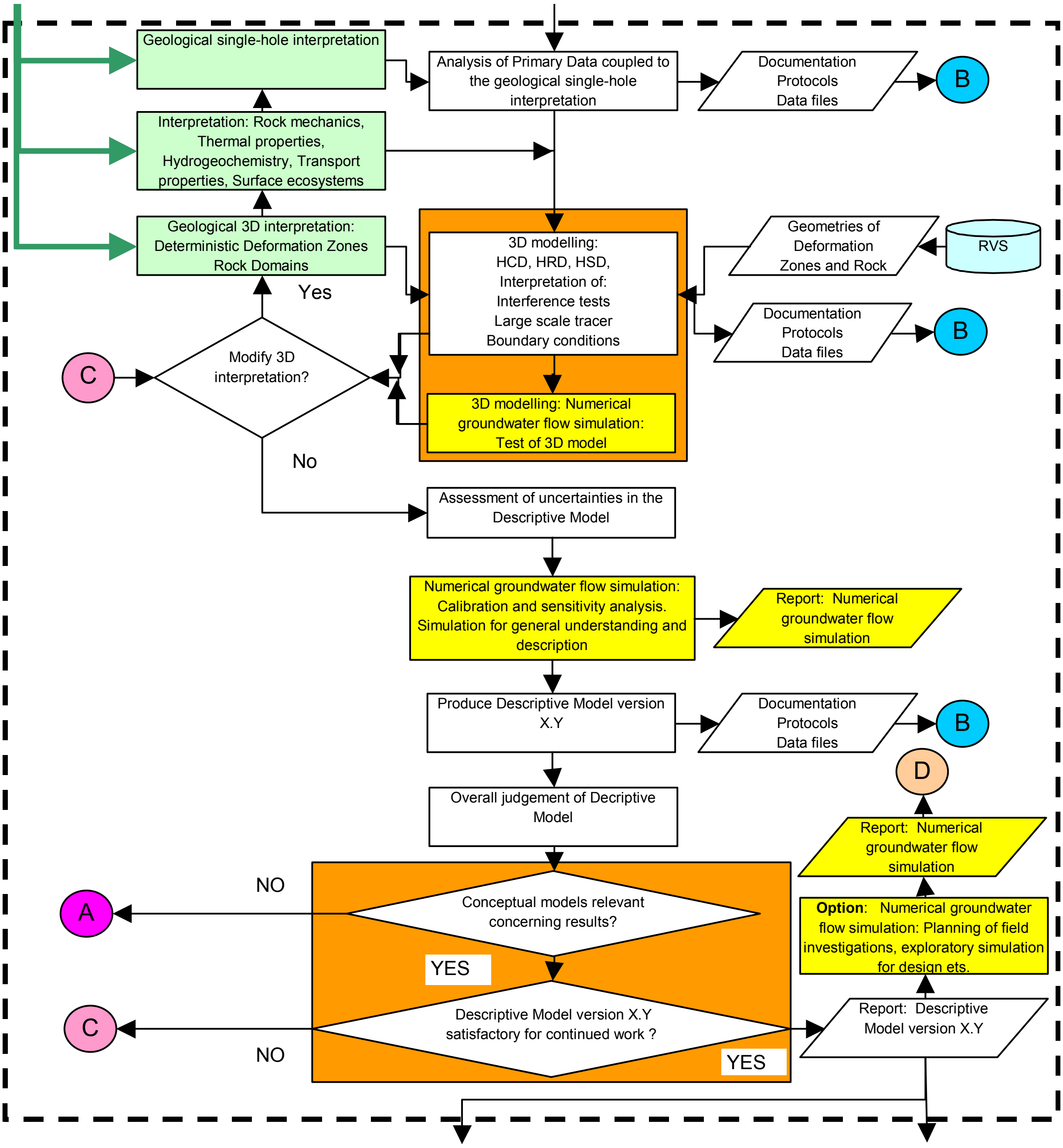


Figure 6-1. *An overview of the general performance of Site Descriptive Hydrogeological Modelling and the interaction with other disciplines. Part of flow chart shown in Figure 1-2 covering the Three-dimensional modelling and Site Description. A, B, C and D show connections in the flow chart in Figure 1-2. A: Conceptual issues call for updating conceptual models. B: Data delivered or data received. C: Descriptive models are up dated because of the interactive and integrated modelling. D: New investigations needed to make the Descriptive models more detailed.*

6.1 Analysis of primary data coupled to geological single-hole interpretation

6.1.1 Primary indication of HCDs and HRDs

The geologist will produce a single-hole interpretation, showing where deterministic deformation zones intersect boreholes in addition to a classification of the rock along each drilled borehole, see Figure 6-2. This is the base for comparison with the hydraulic test results.

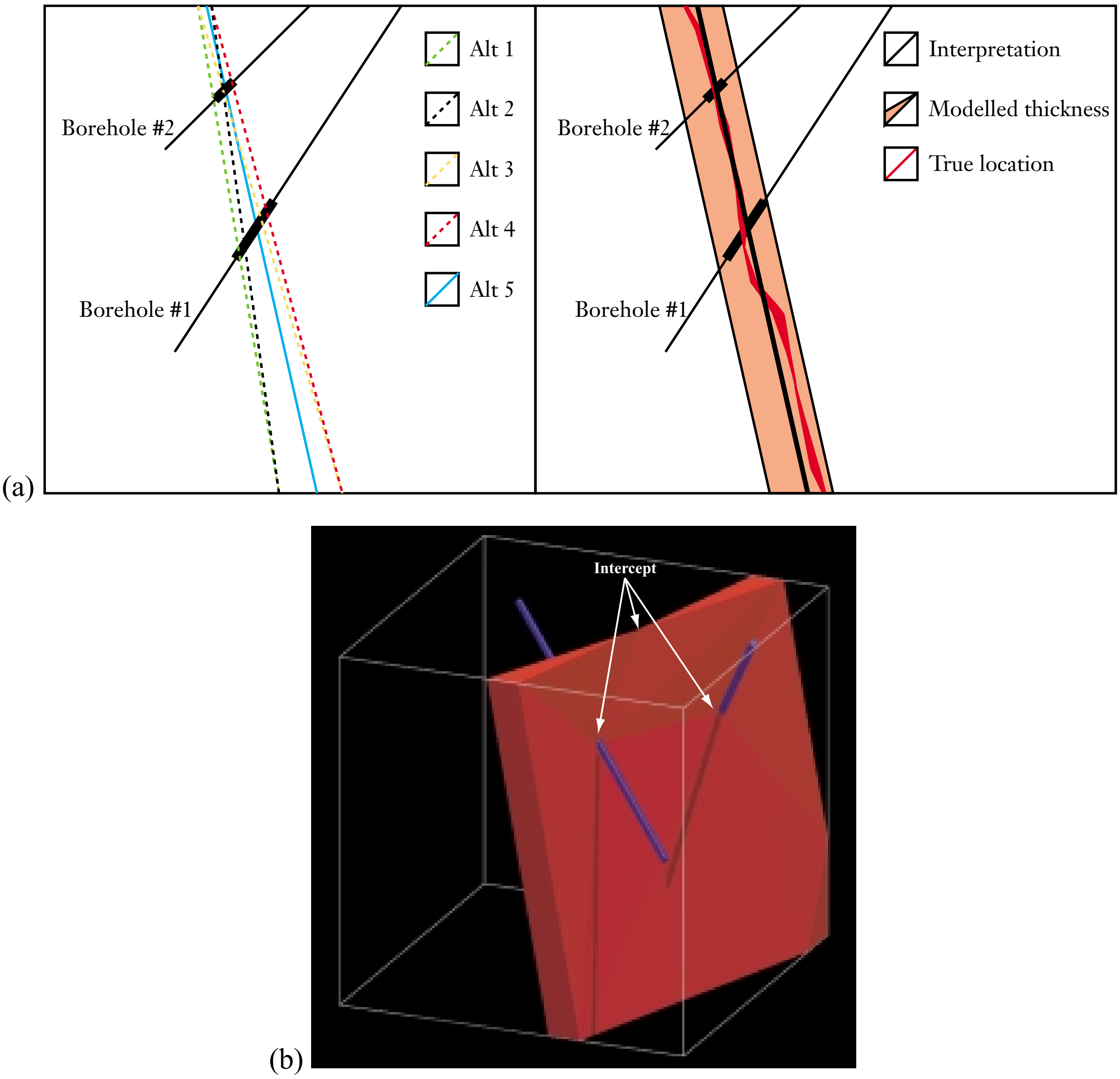


Figure 6-2. Illustration of the 3D interpretation of the borehole intersections of a deformation zon. Possible interpretations of the location of a deformation zone, given surface and borehole intercepts. The thickness of a deformation zone is modelled ((a) right and (b)) to encompass all observations in boreholes and surface and to take into consideration the natural undulation of the structure. /Munier et al, 2003/.

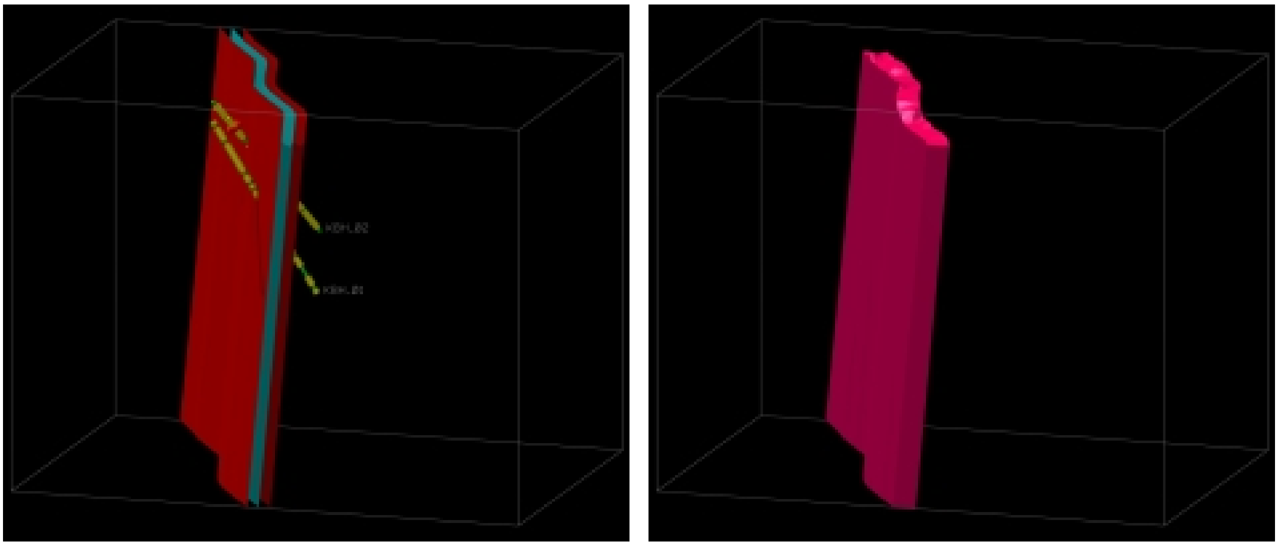


Figure 6-3. *Illustration of the 3D interpretation of the borehole intersections of a deformation zon. Two aspects of a modelled deformation zone. Left: The modelled structural surface (blue) and its normal offsets (red). Right: The modelled thickness. /Munier et al, 2003/.*

The modelling within RVS (Rock Visualisation System) of deformation zones provides a *modelled structural surface* based on the observations of a deformation zone. The modelled deformation zone as a volume, *modelled structural volume*, is based on this surface and the modelled thickness of the deformation zone, see Figure 6-3.

The rock stresses at the site may indicate possible anisotropy of the permeability of the rock mass and are therefore of interest.

The suggested deterministic deformation zones in the model are first scrutinised in the light of the interference test analysis to see if the major deterministic deformation zones in the model presented can explain the responses.

Secondly, the single-hole measurement test results are re-analysed in conjunction with the deformation zone intersection specification, the non-deterministic deformation zone rock and the borehole rock classification. Data are explored with the statistical methods outlined in the following sections.

6.1.2 Primary geostatistical evaluation

The data are re-analysed with univariate statistics based on the geological single-hole interpretation with deformation zone intersections, the non-deterministic deformation zone rock and the borehole rock classification *(Rock types* and *rock segements)*.

The spatial correlation of measurements and observations is analysed with different geostatistical methods. The spatial model of the fracture system with assigned hydraulic properties is described in Section 6.2. In this section the application of geostatistical models directly onto hydraulic observations is outlined.

The correlation between the observations along the boreholes will be studied by means of semivariance modelling. Of interest are the variance, correlations lengths and "hole effects" (periodicity). Spatial data analysis with 3D semivariogram models based on the data from the rock mass may possibly be made, but experience shows that the nugget is high and the correlation range relatively low, thus only giving a spatially correlated field in the immediate vicinity of the boreholes. The support scale can also be expected to vary a great deal between the parameter values, which negates a basic assumption of conventional Kriging. However, other kriging may work. One option is to create a sample of hydraulic conductivities from a groundwater flow model based on a DFN network and then model the semivariance that can be applicable to a SC model (see Chapter 3).

The variance and correlation length for properties of a HCD is of interest but it is difficult to obtain relevant hydraulic data for the analysis. Large-scale variability may in a few cases be analysed based on a few boreholes intersecting the same HCD but small-scale variability has probably be based on a DFN model and analysed as indicated above.

The depth dependency of the HCD and HRD properties will also be explored.

6.2 Evaluation of hydraulic DFN parameters

6.2.1 Introduction

The hydrogeology of sparsely fractured crystalline bedrock is dominated by two fundamental observations; that the main groundwater flow and mass transport are controlled by discrete structural features within the rock mass and that the mean permeability is highly scale dependent and generally anisotropic. As a result of these observations, the hydrogeological model must be capable of reproducing the geometric and hydraulic properties of structural features with a sufficiently detailed resolution for the problem under study. Moreover, it can be assumed that the bulk of the bedrock will not contribute significantly to the total groundwater flow. Discrete Fracture Network (DFN) hydrogeology generally concentrates on an accurate representation of large or more transmissive structural features, sacrificing accuracy in the representation of small or less transmissive structural features. In this case the term "feature" is used, as the type of model described includes both single fractures and large deformation zones. A deformation zone is treated as a "feature" but includes a large number of interconnected fractures.

6.2.2 General concepts

The conceptual model used in the DFN approach assumes that structural features can be modelled as infinitely thin two-dimensional polygons generally called "discrete fractures". Discrete fractures are generated in three-dimensional networks based on the structural geology and the statistical information on the fracturing (trace lines) seen on the outcrops and in the boreholes. The network fractures are of two types; deterministic and stochastic. The deterministic fractures are common to all realisations and conditioned on local observations/measurements, whereas the stochastic fractures are probabilistic and unconditional. The realism of all fracture networks is evaluated both geologically and hydraulically by means of forward modelling and calibration, e.g. by means of comparisons with interference tests conducted in the field.

The key assumptions in the DFN approach may be summarised as follows:

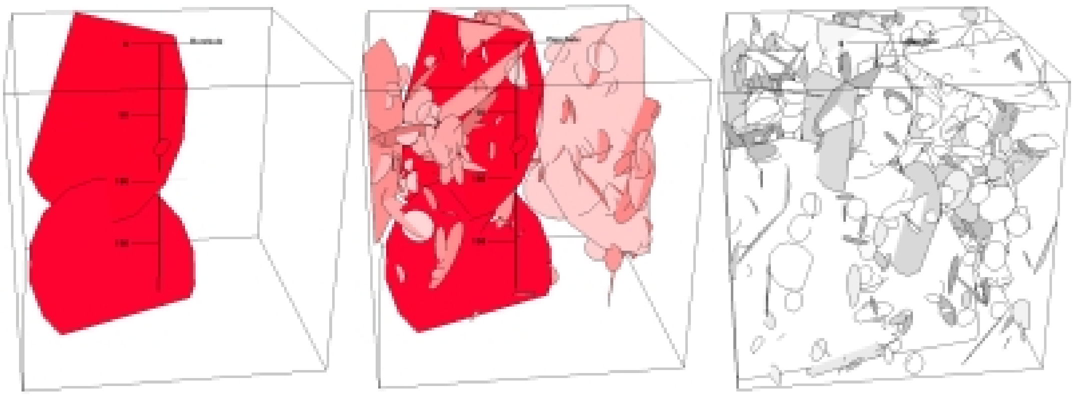
1. Structural features can be modelled by means of two-dimensional polygons (“fractures”).
2. The geometric and hydraulic properties of three-dimensional fracture networks can be derived from structural information such as trace lines (orientation, size, intensity and spatial distribution), and hydraulic tests conducted in boreholes.
3. Unmapped structural features in bedrock can be modelled stochastically by means of Monte Carlo simulations and compared to data from outcrops and in boreholes. The modelling is based on the trace line statistics of those features that have been mapped on outcrops and in boreholes and on the result of the hydraulic tests conducted in boreholes.
4. Groundwater flow through a network of fractures can be described by the same laws pertaining to continuum approaches (i.e. the Navier-Stokes and Darcy equations). The hydraulic properties of the stochastic fractures can be assumed to be independent of (uncorrelated) or dependent on (correlated) the geometric properties (which are probabilistic).
5. Meaningful boundary conditions can be defined and assigned to discrete features at the edges of the model domain and/or at specified locations within the model domain, e.g. along boreholes.

6.2.3 DFN hydraulics

A large part of the work of defining a DFN model is based on trace line statistics and structural geology. This work has been described in detail in the geological modelling /Munier et al, 2003/ and will not be repeated here. However, for the understanding of how groundwater flow is modelled through stochastically generated fracture networks, it is necessary to explain how the trace line statistics can be linked to the hydraulic information from hydraulic measurements and tests in boreholes.

The hydraulic behaviour of crystalline bedrock mainly depends on the transmissivity of the structural features and their connectivity. The conductive portion of a fracture network (as opposed to the complete fracture network) is estimated from hydraulic tests conducted in boreholes. The number of inflow points and their transmissivities are identified by combining different types of measurements such as BIPS logging (optically imaging of the borehole wall), core analysis, difference flow logging and double-packer injection tests. The measurement threshold of the difference flow logging tool and/or the double-packer injection test equipment affects the inferred conductive fracture frequency (CFF), P_{10c}. This means that the lower the measurement threshold, the greater is the conductive fracture frequency indicated by measurements. The natural (open) fractures and the total number of fractures (natural and sealed) are obtained by mapping of the core, see /Munier et al, 2003/. If the measurement threshold is set at nil, the “conductive” fracture frequency should equal the total fracture frequency (TFF), P_{10}, of the natural fractures. It is however not always possible by core mapping to clearly distinguish between natural and sealed fractures, adding an uncertainty to what can be considered as fracture frequency of fractures open for flow.

Figure 6-4 (a) shows a schematic example of the observed conductive fracture frequency in a hypothetical single borehole. An important assumption of DFN hydrogeology is shown in Figure 6-4 (b). The conductive fractures encountered in a single borehole are assumed to be



(a) (b) (c)

Figure 6-4. *(a) Schematic example illustrating three conductive fractures intersecting a hypothetical borehole interval. (b) The conductive fractures in (a) are connected to a larger network of conductive fractures. (c) The conductive fracture network in (b) is merely a subset of the entire fracture network.*

connected to other conductive fractures in the rock mass. It is important to note, however, that the degree of connectivity will vary in space and between realisations. That is, the conductive fractures in a single borehole do not necessarily connect to all conductive fractures in the rock mass as illustrated in Figure 6-4 (b).

Based on the experience of investigations carried out at SKB's study sites, including Äspö HRL, it may be concluded that a measurement threshold of the order of (1 to 5) $\cdot 10^{-11}$ m^2/s is sufficient to model the body of the groundwater flow in the rock mass between major fracture zones. The corresponding conductive fracture frequency for such a low range measurement threshold is nevertheless merely a fraction of the total fracture frequency. The latter is schematically illustrated in Figure 6-4 (c). However, probably higher threshold values can be accepted for large-scale groundwater flow models.

A difference flow log with a high resolution (step length ~ 0.1 m) can pick up individual flow features above a given inflow measurement threshold and thus directly provide input to a transmissivity analysis. A difference flow log with a lower resolution (step length ~1.0 m) and double-packer injection tests provides transmissivity information over a section length that can include several flow features. The following method can be used in such cases /FracMan, 1996/.

The transmissivity T of a single fracture in a 1 m long borehole section in an otherwise impermeable rock is equivalent to the conductivity K of the same 1 m long borehole section in continuous porous material. The transmissivity distribution and the frequency of conductive fractures from packer test data can be determined by the Osnes approach, described by /Osnes et al, 1988/. The method assumes that the fracture network transmissivity of a borehole section is equal to the sum of the transmissivities of the conductive fractures that intersect that test zone:

$$T_1 = \sum_{j=1}^{n_i} T_{ij}$$

where T_i is the apparent transmissivity of the *ith* packer interval, n_i is the number of conductive fractures in the *ith* interval and T_{ij} is the transmissivity of the *jth* conductive fracture within the *ith* interval. Within any given interval, the number of conductive fractures, n_i, can be assumed to be a random number defined by Poisson distribution /Benjamin and Cornell, 1970/:

$$f_n(n) = \frac{\overline{n}^n e^{-\overline{n}}}{n!}$$

Where $\overline{n}$ is the Poisson process rate, which is equal to the expected value of n. The conductive fracture frequency is given by $f_c = n/L_i$, where L_i = the length of the test zone.

This approach assumes that the fractures are evenly distributed along the borehole. This is not always the case and should be carefully checked before any evaluation.

The distribution of fracture transmissivities is assumed to be independent within each packer interval with a given distributional form. The distribution of T_i is the sum of number of random events and is therefore a compound Poisson process /Feller, 1971/. In this approach, the mean number of fractures in a given interval is defined by the Poisson distribution rate parameter, n, and the distribution of fracture transmissivities T_{ij} can be described by a log normal distribution with a mean and standard deviation (m_{logT} and s_{logT}).

For any given set of parameters describing the distribution of fracture transmissivity $f(T_{ij})$ and conductive fracture frequency f_c, the distribution of packer interval transmissivities $f(T_i)$ can be found by means of Monte Carlo simulation, with the best fit value being identified by a simulated annealing search routine. If the flow log data do not permit a direct evaluation of the conductive fracture frequency f_c, an initial guess is made, and the Monte Carlo simulation process is run until there is a good match with either data observed by Kolmogorov-Smirnov (K-S) or with Chi-Squared (χ^2) statistics.

Simulated intervals that contain no conductive fractures or that have T_i values of less than $T_{threshold}$, the lowest threshold transmissivity that can be reliably measured in the field, are assigned a transmissivity equal to $T_{threshold}$.

The intensity and transmissivity distributions for the conductive fractures are then estimated by finding the best match between the observed distribution of packer interval transmissivities $f(T_i)$ and the distribution of test zone transmissivities found by simulation in respect of a given fracture frequency as well as single-fracture transmissivity distributions established by comparison with Kolmogorov-Smirnov (K-S) or Chi-Squared (χ^2) statistics.

The values of n, $\mu_{log\,T}$ and $\sigma_{log\,T}$ that provided the best K-S or χ^2 are taken to be the best estimates of these parameters.

The DFN parameters for the geometry and transmissivity distribution are conveniently presented in table form to facilitate further use of the data, cf Table 6-1.

Table 6-1. Geometric and hydraulic parameters for a typical DFN model /from Stigsson et al, 2001/.

Parameter	Used data	Data from	Reference
Orientation	Set Strike Dip K 1 219 83.7 4.84 2 127 84.2 8.35 3 20.6 6 8.33	Pilot and Exploratory holes	This report
Size	Set mean Std dev 1 2 2 2 8 2 3 5 4	TBM tunnel	Follin & Hermanson (1996)
Location model	Poisson distributed Enhanced Baecher	TBM tunnel	Follin & Hermanson (1996)
Conductive intensity, P_{32c}	0.71	Exploratory holes 1 m and 3 m test	This report
Transmissivity distribution $\log_{10}(T)$	Set mean Std dev Upper trunc 1 –11.5 2.30 –5 2 –10.3 2.07 –6 3 –11.6 1.47 –7	Pilot and Exploratory holes	This report
Model size	100 x 175 x 100 m (North, East, Up)		
Centre point in Äspö96 Co-ordinates	North = 7271 m East = 1899 m Z = –448 m		
Outer boundary conditions	Specified head boundary	site scale model	Svensson (1997)
Inner boundaries	Tunnels as head simulating atmospheric pressure p = 0. Boreholes, no flow or hydraulichead according to performed tests	Performed tests	Gentzschein (personal communication 1998) and Forsmark and Rhén (1999)

6.3 3D Modelling

The main target sizes are a Regional Site Descriptive model and a Local Site Descriptive model. In principle, both modelling scales have to be updated in each phase of the investigations. However, it is likely that the changes in the Regional Site Descriptive model will be reduced as the Site Investigation proceeds and it may reach a situation, where the geometric framework and rock properties are only updated in the Local Scale model. The same may apply to the groundwater flow model in the Regional model domain, which will not be updated for each investigation phase if it is considered that the Regional model domain groundwater flow model can provide proper boundary conditions for the Local Scale model.

The integrated 3D modelling work covers analysis of primary data as well as groundwater flow simulations and these are strongly connected. In this report, it is dealt with in two sections; 6.3 and 6.4. However, each time the descriptive model is updated, the geometry and properties of the hydraulic domains must first be defined in order to provide input for a revised groundwater flow model. The base for the groundwater flow model is the geometric models of deformation zones and rock domains developed within RVS (Rock Visualisation System). Figure 6-5 illustrates the geometry of modelled deformations zones at Simpevarp model version 0. It may however be useful to partly update a groundwater flow model for the purpose of testing some hypotheses at an early stage of the 3D modelling process.

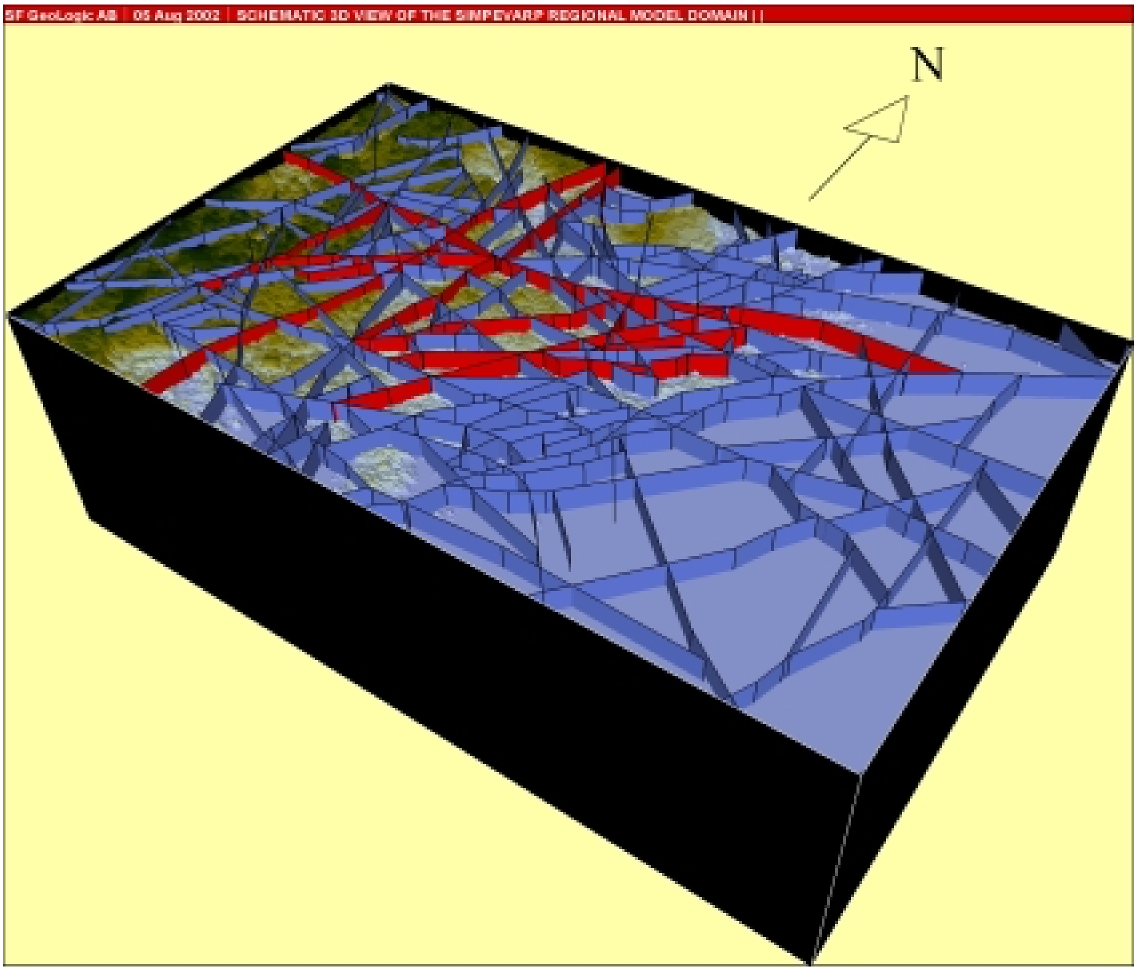


Figure 6-5. *The geometry of modelled deformations zones at Simpevarp model version 0.*

6.3.1 HCD, HRD and HSD: Geometry and properties

Primary indications of HCDs and HRDs and the statistical evaluation of data, as described in Sections 6.1 and 6.2, form the hydrogeological foundation for the disciplines' integrated analysis of the deterministically defined deformation zones and the suggested rock domains. The 3D integrated analysis may lead to changes in the geometrical model of the deterministically defined deformation zones and the rock domains. Some of the univariate statistics and geostatistical analysis may have to be updated as a result.

Interference tests and large-scale tracer tests

Measured interferences (pressure responses in surrounding boreholes) during drilling, hydraulic tests of a relatively short duration (for example 100 m test-scale test during the drilling of core holes, hydraulic tests in percussion boreholes etc) may provide useful information for the interpretation of the general pattern of hydraulic anisotropy or specific fracture zones. However, a study of the responses of well-controlled interference tests provides the most reliable information for the examination of (some of) the fracture zones in the geological model. The responses measured during an interference test may indicate how the geometrical model should be modified.

The limitations of interference tests is that, if there is little contrast in hydraulic properties between a hydraulic feature and the rest of the rock mass, or if the permeability of the feature is low, the responses in the observation sections may be insignificant or non-conclusive. In such a case, the geological interpretation of the geometry and the single-holes tests form the base for assigning fracture zone properties.

If several boreholes intersect a deformation zone as shown in Figure 6-2 it may be possible to interpret the storage coefficient and to study the large-scale variability within the zone.

HCD property assignment

The thickness (total zone width, see Figure 3-7) of the deformation zone is defined in the geological description of a specific zone. The geological interpretation provides an estimate of the zone thickness at each borehole intersection (Calculated Thickness of Structure (CTS)) and modelled zone geometries within RVS. The geometric elements describing the deformation zones that can be exported from RVS: Modelled Structural surface (MSS), a 2D-element and Modelled structural volume (MSV), a volume describing the deformation zone, see Figure 6-3. The uncertainty of the geometry of the deformation zone is represented by a volume called Modelled uncertainty of Deformation zone, see Figure 6-14.

The first step is to use single-hole tests and the geometric geological model to analyse the sections of the boreholes where the deterministic deformation zones are expected to intersect. Hydraulic tests of longer duration (and subsequently a longer evaluation period) straddling a specified fracture zone are generally considered to provide a more representative estimate of the average properties of the zone if the zone is much more permeable than the surrounding rock mass.

If no hydraulic tests have been performed in a specific zone, tentative hydraulic properties are assigned to the fracture zone based on the geological description of the fracture zone and the general knowledge of the hydraulic properties of neighbouring fracture zones. The univariate statistics of the HCDs properties as well as the depth dependency is presented as a base for the assignment of properties to suggested deterministic deformation zones where no hydraulic tests have been performed.

If several boreholes intersect a HCD, it is possible to obtain a rough view of the large-scale variability. Geologists can to some extent describe the small-scale variability, internal structure and the character of the fracture fillings within a HCD. Some generalised types of deformation zones can possibly be generated with the DFN approach, based on the geological description of the deformation zones. The variability within the various types can then be studied as outlined in Section 6.1.

HRD property assignment

The geometric geological model showing the different sections of the boreholes where the rock domains are expected to intersect is used to classify single-hole test results. Analysis of the data is made to see whether some of the rock domains should be further subdivided or if they can be grouped together into HRDs. Univariate statistics are presented for each HRD and measurement scale. The geostatistical analysis, including a general analysis of the depth dependence, is also presented. A decision is taken as to whether the DFN requires updating.

Interference tests generate responses in HCDs as well as HRDs. The heterogeneity of HRDs applied as stochastically distributed properties in HRDs in groundwater flow models makes it difficult to compare observations to simulations. However, the results from several realisations of the stochastic field can be compared to the observations, and the assigned correlation between transmissivity and the storage coefficient (or hydraulic conductivity-specific storage) can be assessed.

Boundary and initial conditions

Boundary and initial conditions are needed for the numerical simulation. Measurements of levels of lakes and the sea as well as the topography are well-defined upper boundary conditions. Observations of run-off rates are important for the understanding of the water balance within an area. The run-off rates are used to define the mean effective precipitation (specific runoff) in the numerical modelling. Measurements of piezometric levels and TDS (or EC) are important for the assessment of the boundary and initial conditions. The pressure and TDS distribution in the soil deposits and rock mass can only be measured at relatively few points. Data will suggest suitable boundary and initial conditions but must be tested by the numerical model. Observations of simulated pressures and TDS will then be compared to measured pressures and TDS. It is foreseen that simulations of the groundwater flow since last glaciation will be a part of the simulations to test appropriate present day conditions and concepts for the property assignment.

6.4 Numerical groundwater flow simulations: Test and calibration of the 3D model

This section describes the framework associated with the testing and application of 3D numerical groundwater flow models in support of the development of a Hydrogeological Site Descriptive Model. The overall objective of 3D numerical groundwater flow modelling within the SKB Site Investigation Programme is to assess the conceptual understanding of the physical hydrogeological system and, in particular, to assess the uncertainty in the Site Descriptive Hydrogeological Model. This is accomplished by numerical simulation, i.e. the complete execution of a groundwater modelling computer code including input and output.

The entire groundwater flow modelling process is shown in Figure 6-6, which is a part of the overall modelling process shown in Figures 1-2 (and also in Figure 6-1). Figure 1-2 shows the overview of the Site Descriptive Hydrogeological Modelling process and the interaction between Hydrogeology and the other geoscientific disciplines (Geology, Rock Mechanics, Hydrogeochemistry, Thermal Properties, Surface Ecosystems, and Transport Properties). 3D numerical groundwater flow modelling comes into play in the section entitled “Integrated evaluation and Site description”. Among the other disciplines, the Site Descriptive Geological Model is the most important for integrated evaluation from a hydrogeological point of view.

Numerical groundwater flow codes that may be used are shortly described in Appendix 2.

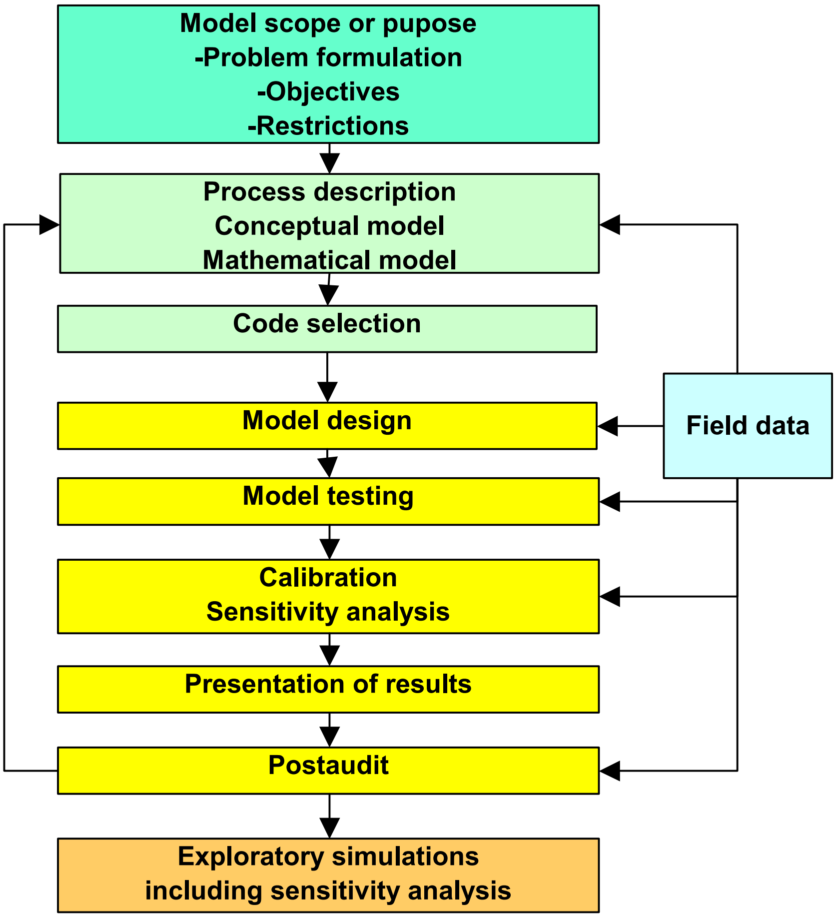


***Figure 6-6.** An overview of the general performance of groundwater flow simulations as a part of the Hydrogeological Modelling in 3D.*

6.4.1 Procedure

The use of numerical simulation within the SKB Site Investigation programme is twofold, testing and application, where the latter requires a substantial amount of the former. In brief, the application of a numerical groundwater flow model involves seven basic steps to achieve an acceptable representation of the physical hydrogeological system and to document the results of the model study. These primary steps include the following:

- Task Description.
- Technical audit of conceptual assumptions used for the numerical groundwater flow models.
- Model design (construction) of a geology based 3D numerical flow model.
- Model testing of geometric interpretation alternatives.
- Hydraulic calibration and sensitivity analysis.
- Simulation for general understanding, description and presentation.
- Presentation of results (documentation).

These steps are designed to identify and document the understanding of the flow system, the implementation of the descriptive geological-hydraulic model in a mathematical framework, and the degree of uncertainty in the calibrated model. The steps should generally be followed in the order in which they appear above; however, there is often a significant iteration between steps. All steps are required for a model that simulates measured field conditions. In the following sections, each step is described in greater detail.

6.4.2 Task Description

As described in Table 1-1, numerical groundwater flow models will be used on two scales, regional and local, within the SKB Site Investigation Programme, where the local model domain encompasses a subvolume of the regional model domain. In either case, the Site Descriptive Hydrogeological Model emanates from a geometric framework common to all geoscientific disciplines, i.e. the difference is mainly in the size of the model domain and in the geometric resolution of the mesh of the numerical model rather than in the underlying concepts and data.

Regardless of scale and version, every project that involves numerical simulations will be specified by means of a *Task Description* (TD). A Task Description lists SKB's general and specific objectives for the numerical simulations, and specifies a minimum level of quality assurance in the model setup and expected output. Figure 6-7 shows a tentative example of a Task description layout.

Upon delivery of a Task description, SKB will commence a dialogue with the modellers in order to compile an *Activity Plan* if the TD is considered not detailed enough. If accepted and signed by SKB, the execution of the Activity Plan or TD, including deviations, is in accordance with SKB's Quality Assurance System in line with other SKB activities.

While executing a particular Task Description, it is important to recognise that unforeseen interpretations may arise as a result of the integrated evaluation of data. Unforeseen interpretations will be analysed by SKB and addressed accordingly. For instance, a new interpretation may need to be hydraulically tested by means of numerical simulations. In such a case, depending on the complexity of the new interpretation, the testing can either be incorporated into the onging modelling Task Description or treated separately by means of another Task Description.

6.4.3 Technical audit of numerical flow models

As indicated in the example of a Task description shown in Figure 6-7, the application of a numerical groundwater flow model includes a technical audit of the numerical modellers' treatment of:

- Conceptual representation.
- Dimensionality.
- Discretisation.
- Initial and boundary conditions.
- Hydraulic properties.

	Task Description (TD)
Task title	Groundwater flow simulations for the Simpevarp regional model area, v1.2
Date	2003-xx-yy
Version	1.xx
Author(s)	NN
Narrative	Model test of recharge rate and hydraulic connectivity between the cored boreholes KSM01 – KSM02.
Model version	Site Descriptive Hydrogeological Model 1.2
Objectives	The objective of this task is to support the update of version 1.1 of the Site Descriptive Hydrogeological Model (SKB R-0x-xx). The numerical modelling should be based on the 1.2 version Site Descriptive Geological Model alternatives A – C (SKB R-0y-yy). For each one of these three variants, the numerical modelling should study the specific discharge rate (Darcy flux) to the bedrock at z = –500 m and the hydraulic connectivity between the cored boreholes KSM01 – KSM02.
Scope	Three model alternatives, A – C shall be modelled and analysed. With regard to forthcoming safety assessments, the documentation of the simulation results must allow for a subsequent calculation of Darcy fluxes at repository depth, advective travel times and F-factors along the simulated pathways. Regarding the repository layout, a hypothetical design may be used at this point, but the assumptions made must be approved by SKB. From an engineering point of view, simulations of drawdown will probably be used to test various design issues.
Modelling constraints	Data from single-hole measurements performed in the following boreholes must be used in the definition of the hydraulic properties: HSM01 – HSM02 and KSM01 – KSM02.
Expected output and delivery	The documentation of the numerical simulations should focus on a hydraulic comparison between the three variants. The planned date for an oral presentation is 2003-xx-yy and the expected deadline for a draft report is 2003-xx-yy.
Modelled processes	Shoreline displacement. Transient, saturated variable-density flow. Particle tracking.
Model domain	Simpevarp area: Coordinate system: (X: Easting, Y: Northing): RT90 2.5 gon W, Elevation (Z): RHB 70, unit m, Regional model, (X,Y): (1539000, 6373000), (1560000, 6373000), (1539000, 6360000), (1560000, 6360000), Elevation Z 50 / -2200 Topography: 50m grid size used for the "super regional" models.
Discretisation	100 m x 100 m in the horizontal directions and up to 100 m in the vertical direction
Initial condition	Initial pressures and salinities are set according to the assumption made prior to version 1.1. No flow boundary conditions are assumed for the lateral sides and the bottom side of the model domain, except for the lateral side facing the Baltic Sea.
Boundary conditions	Specific runoff and TDS=0 are used for the top boundary, except under the Baltic Sea where the water pressure and the concentration at the sea floor is set to reproduce changing water salinities/depths due to the shoreline displacement.
Properties	Background conductivities of the regolith (soil) deposits and the upper section of the bedrock are identical to version 1.1. Remaining parts of the bedrock are modelled with the stochastic continuum approach. Deterministic fracture zones are treated separately.
Calibration targets and performance measures	Minor fracture zone transmissivities and rock mass conductivities between major fracture zones are updated according to the result of the Model testing in HSM01 – HSM02 and KSM01 – KSM02. Simulated flow rates in streams and simulated lake water elevations are compared with measured data.
Date	Signature
2003-xx-yy	NN, SKB
2003-xx-yy	NN (Model team XX), NN (Model team YY)

Figure 6-7. *Tentative example of a Task Description layout.*

Spatial dimensionality is determined by the modelling objectives and by the nature of the groundwater flow system. Unless otherwise specified, all numerical flow modelling within the SKB Site Investigation programme should be performed in three dimensions (3D).

Temporal dimensionality is the choice between steady state or transient flow conditions. In principle, steady-state simulations produce average or long-term results and require that a true equilibrium case is physically possible. Transient analyses are typically performed when boundary conditions vary over time (e.g. due to shoreline displacement) or when study objectives require solutions at more than one point in time (e.g. pumping tests). Steady state or pseudo-steady state (within a specified volume and time, with constant-rate pumping or injection, the piezometric-level changing rates are the same and can be treated as local steady state conditions) can however be justified to test connectivity's and make local calibrations.

Traditionally the *conceptual representation* of 3D groundwater flow through sparsely fractured rocks is numerically modelled as flow through 3D cubes (Stochastic Continuum) or 2D planes (Discrete Fracture Network). The choice of conceptual representation depends on the nature of the input data and the objectives of the numerical simulation. In some cases, different conceptual representations may be run in parallel as a means of assessing the relative conceptual uncertainty, e.g. in performance assessment modelling and in the handling of saline groundwater.

Spatial discretisation is a critical step in every model construction process. An incorrect choice of the spatial discretisation may not only affect the possibility of representing the heterogeneity of the input data, e.g. the spatial variability of detailed injection tests between packers in boreholes, but also the numerical stability. For obvious reasons, it is not possible to treat recordings from the field without some kind of averaging if the measurement scale is smaller than the discretisation. In order to establish the presence of numerical errors, the modellers should carry out tests with at least one other spatial discretisation. The results should be fully documented in the model report.

Temporal discretisation is the selection of the number and size of time steps for the period of transient numerical simulations. The temporal discretisation is particularly important in simulations dealing with mass transport (e.g. salt). Depending on the size of the spatial discretisation used, there may be numerical constraints on the maximum time-step, i.e. the size of the numerical time-stepping scheme, due to numerical instability. In order to assess if numerical instability is present in the temporal discretisation used, the modellers should carry out numerical tests with another numerical time-stepping scheme. The results should be fully documented in the model report. It is also recommended that the modellers ensure that the Courant-criterion and the Neumann-criterion are fulfilled in the early stages of model setup. The Courant-criterion states that a greater mass cannot leave the cell via advection during the time interval $[t, t+\Delta t]$ than is inside the cell at the beginning of the time interval. The Neumann-criterion states that concentration gradients cannot be reversed by dispersion-diffusion fluxes alone /Anderson and Woessner, 1992/ . Further information on various numerical criteria for numerical groundwater modelling can be found in the groundwater literature.

Initial and boundary conditions. Initial conditions provide a starting point for transient simulations. Steady-state models do not require initial conditions. Initial conditions consist of pressures (or hydraulic heads) and concentrations (e.g. salinities) for each model node at the beginning of the simulation. Initial conditions may represent a steady-state solution obtained from the same model. In order to assess the effect of the initial conditions on the results, the modellers should perform numerical tests with a different setup of initial conditions. The results should be fully documented in the model report.

All numerical groundwater flow models require that a boundary condition is assigned to every model node along the boundary surface of the model domain and to all internal sources or sinks (e.g. pumping tests, tracer tests, saline groundwater). Boundary conditions relevant to the SKB Site Investigation Programme fall into one of the following four categories: specified pressure and concentration, specified fluid flux and mass flux, mixed conditions, and free surface boundary (water table). It is desirable to include only natural hydrologic boundaries as boundary conditions in the model setup. If the specification of artificial boundaries at the edges of the model domain is unavoidable, the modellers should perform numerical tests to test the impact of the artificial boundaries to ensure that these are sufficiently remote from the target area. The results should be fully documented in the model report.

Hydraulic properties include the water-conducting capacity and storage characteristics of the flow system. The flow system of interest is both porous (HSD) and fractured (HCD and HRD) and the conceptual model must address this complexity, e.g. the hydraulic interaction between these three domains. Examples of hydraulic properties include transmissivity and storativity, hydraulic conductivity and specific storage coefficient as well as the specific yield. Hydraulic properties may be homogeneous or heterogeneous throughout the model domain. Certain properties, such as hydraulic conductivity, may also have directionality, i.e. the property may be anisotropic. It is important to document the field and laboratory measurements of these properties in order to set bounds or acceptable ranges for guiding the generation of stochastic realisations (Monte Carlo simulations) and model calibration.

6.4.4 Model design – construction of a geologically based 3D numerical flow model

The construction of a geologically based 3D numerical groundwater flow model depends on the modelling approach used. The two main approaches are the stochastic continuum approach and the discrete fracture network approach, see Chapter 3 and Figure 3-4. The hydraulic parameters for the identified HSD, HRD and HCD hydraulic domains, see Figures 3-2 and 3-3, associated with the two modelling approaches are described in Sections 3.2–3.6. The geometric elements are exported from RVS to the numerical model. Regarding HCD it is an option to implement each HCD as a surface or a volume, see Figure 6-8 and Section 6.1.1.

If the numerical modelling is based on the stochastic continuum approach, it is important that the modellers thoroughly document, among other things, the management of scale, i.e. the coupling of hydraulic conductivity data (measurement scale) and the chosen resolution of the numerical model (support scale, discretisation). The documentation must also make it clear the extent to which Monte Carlo simulations are conditioned, e.g. the matching of measured borehole packer test data, and the statistical evidence for the use of autocorrelation in the Monte Carlo simulations.

If the numerical modelling is based on the discrete fracture network approach (or a hybrid of such an approach) it is important that the modellers thoroughly document, among other things, (*i*) the rationale for dividing the structural geology into deterministic and stochastic features (e.g. deterministic fracture zones and stochastic fractures), and (*ii*) the coupling (if any) of the geometric and hydraulic properties of the modelled features. It must also be clear from the documentation to what extent the geometry of the fracture network realisations is based on calibration (deterministic features) and conditioning (stochastic features), cf Section 6.2.

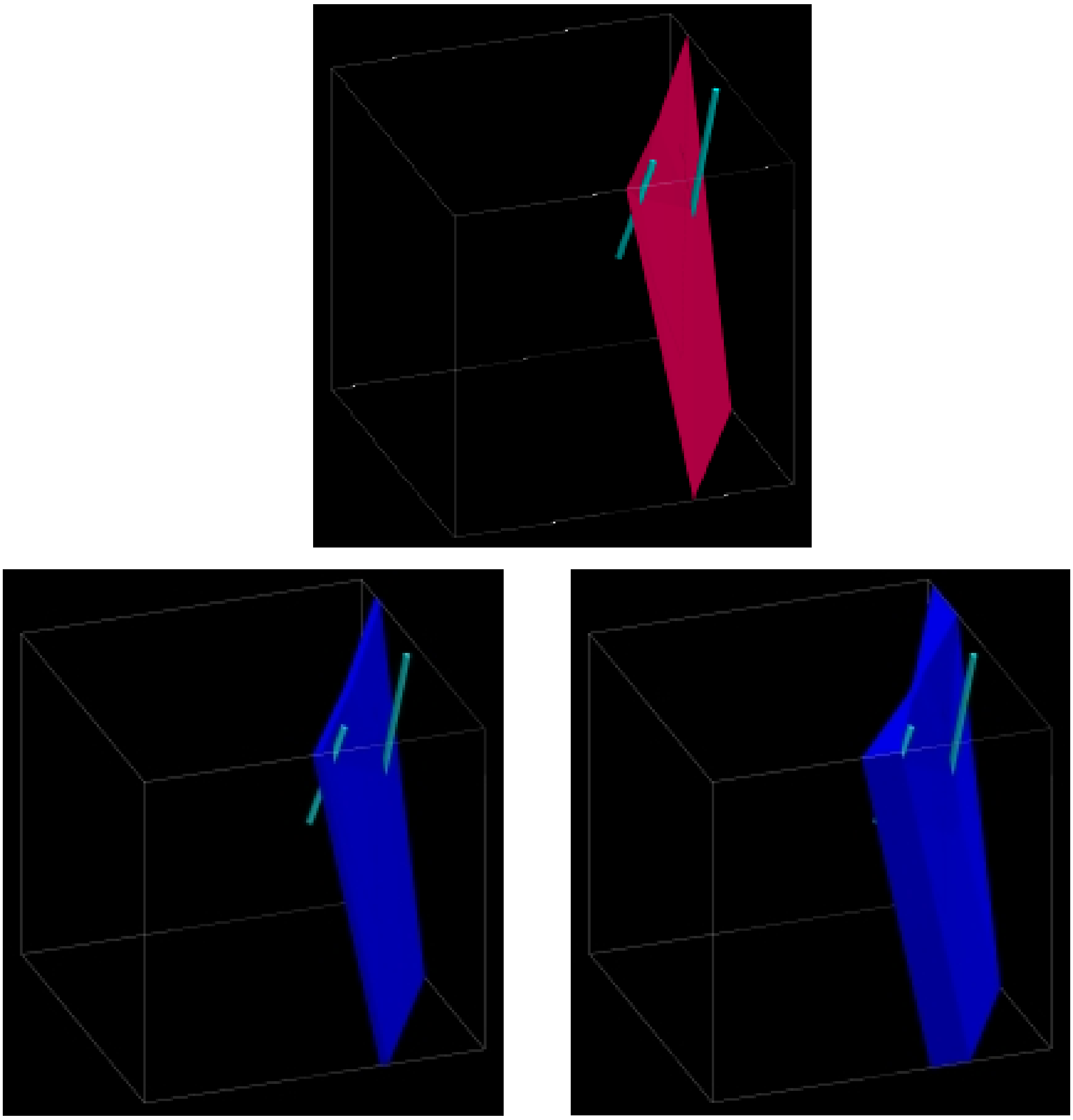


Figure 6-8. *Schematic view of the geometric elements describing the deformations zones exported from RVS. Top: Modelled Structural surface (MSS). Bottom left: Modelled Structural volume (MSV) with constant thickness. Bottom right: Modelled Structural volume (MSV) with varaible thickness. /Munier et al, 2003/.*

6.4.5 Model testing of alternative geometric interpretations

The Site Descriptive Geological Model will continue to develop for the duration of the investigations. The reason for this is twofold; the size of the model domain and the geometric-hydraulic complexity of the fractured medium. At the start of the Site Investigations, there will be a great deal of uncertainly surrounding the Site Descriptive Geological Model. In due course, a few more or less "deterministic" geometric interpretations may be defined as more data emerge. At this point, *Model testing* plays an important role as a means of investigating which of the alternatives are hydraulically unreasonable and which are not. Ideally, one would hope for only one valid geometric interpretation, which would suggest that the process of

Model testing is capable of finding a unique solution. It should be noted, however, that Model testing is an inexact method that allows one to disprove but not to prove a given geometric interpretation. Hence, the ultimate “one and only” geometric interpretation is merely a working hypothesis, which over time will lend itself to alternative geometric interpretations whenever more data are gathered or the level of detail is increased. In this iterative process, Model testing has a clear objective – to demonstrate that our understanding of the modelled flow system is sufficiently credible. Possible performance measures that may be used for a quantitative evaluation of the Model testing process are discussed in the following section.

Besides the geological structural model the hydrogeochemical data (mainly TDS) may also give indications of how the geometry HCD should be to get a similar hydrogeochemical response as observed in the field.

6.4.6 Hydraulic calibration and sensitivity analysis

Whereas Model testing is concerned with geometric interpretation alternatives, *hydraulic calibration* of a groundwater flow model is the process of adjusting hydraulic parameters, boundary conditions, and initial conditions within reasonable ranges to obtain a match between simulated and observed geohydrological calibration targets such as pressures, flow rates, concentrations etc. Automatic inverse techniques are growing in popularity among specialists, but in practice, model calibration is frequently accomplished through trial-error adjustment of the model’s input data to match the observations. The range over which model parameters and boundary conditions may be varied is determined by data presented in the descriptive model. In the case where parameters are well characterised by field measurements, the range over which that parameter is varied in the model should be consistent with the range observed in the field.

The degree of agreement between model simulations and field measurements can be quantified using statistical techniques. Ideally, criteria for an acceptable calibration should be established prior to starting the calibration. Among the various criteria that can be found in the literature, the following calibration criteria are frequently used (*r* is the residual of the simulated value of the variable *x* minus the observed value of the same variable):

Normalised mean error	$\mathrm{NME}=\mathrm{ME}/(x_{\mathrm{MAX}}-x_{\mathrm{MIN}})$	$ME = \frac{1}{n}\sum_{i=1}^{n} r_i$
Normalised mean absolute error	$\mathrm{NMAE}=\mathrm{MAE}/(x_{\mathrm{MAX}}-x_{\mathrm{MIN}})$	$MAE = \frac{1}{n}\sum_{i=1}^{n} \lvert r_i \rvert$
Normalised root mean squared error	$\mathrm{NRMR}=\mathrm{RMR}/(x_{\mathrm{MAX}}-x_{\mathrm{MIN}})$	$RMS = \left(\frac{1}{n}\sum_{i=1}^{n} r_i^2\right)^{0.5}$

The above can be applied to measurements of piezometric pressure, level of water table, TDS in borehole sections, runoff rates and Darcy fluxes estimated from dilution tests and can also be considered as one type of performance measures, see below.

Hydraulic calibration, as used in its classic context, tacitly assumes that the underlying geometric framework, which constitutes the platform for the definition of hydraulic domains in the hydrogeological description, is correct. It is important to emphasize that hydraulic calibration in the classic hydrological context is difficult to accomplish in fractured media. As long as significantly different alternative geometric interpretations exist, hydraulic calibration in its classic context makes no sense. In such a case, *Model testing* is a more appropriate term for what is accomplished hydraulically (cf the previous section).

Hydraulic sensitivity analysis is the procedure by which the impact of variability or uncertainty in model inputs on the hydraulic performance of the calibrated model is quantified and evaluated. If a small change in the hydraulic setting of any of the model inputs drastically changes the model's degree of hydraulic response, this means that the calibration sensitivity is high. Typically, one or a few *performance measures* (or *objective functions*) are defined at the start of the modelling, for which the calibration sensitivity of the model is evaluated. In a pure hydrogeological context, the performance measures may be formulated by comparisons with measured data, e.g. the position of the interface between fresh and saline groundwater in boreholes, the response of executed pumping tests and tracer tests, runoff rates, distribution of recharge and discharage areas (partly measurable), etc. Performance measures may also be flow pattern from recharge to discharge areas and Darcy fluxes at different depth for comparison between models. The performance measures may also be formulated for the transport assessment measures of interest, e.g. advective travel times between a tentative repository and the biosphere, Darcy fluxes at repository depth, flow path resistances (F-factors), distribution positions and patterns at discharge locations for particles released at repository depth etc. From a design perspective, the performance measures may be formulated in terms of the effect of different layout solutions on the inflow rates to the canister holes, the shape and magnitude of the drawdown in the rock and in the overburden during construction and operation, etc.

6.4.7 Simulation to achieve a general understanding, description and presentation

An important part of the confidence building in the construction of numerical flow models is to simulate the hydraulic behaviour of the numerical groundwater flow model and to communicate the results. The main objectives of flow simulations are:

- to demonstrate the present understanding of the modelled flow system,
- to test and describe the effects on the modelled flow system of various assumptions, and
- to provide input for safety analysis and repository design modelling.

6.4.8 Presentation of results – documentation

The purpose of the model report is to communicate findings, to document the procedures and assumptions inherent in the study, and to provide detailed information for peer review. The report should be a complete document allowing reviewers and decision makers (SKB) to form their own opinion as to the credibility of the numerical flow model. Furthermore, the report should be detailed enough for an independent modeller to duplicate the model results (traceability). Finally, the model report should describe all aspects of the modelling study outlined in Section 6.4. A sample table of contents for a groundwater modelling report is shown in Figure 6-9. The original example comes from a standard guide on the application of groundwater flow models published by the American Society for Testing and Materials /ASTM, 1999/.

6.4.9 Examples of modelling results

The implemented geometries, properties and boundary conditions in a numerical code form the “Groundwater flow model”, see Figure 6-10. The Groundwater flow model can then be used to perform simulations with natural (undisturbed) conditions and interference tests. These simulations will primarily indicate if the assigned HCD and HRD properties are reasonable.

1 Introduction
1.1 General Setting
1.2 Study Objectives

2 Conceptual Model
2.1 Hydrogeological System Framework
2.2 Groundwater Flow System
2.3 Hydrologic Boundaries
2.4 Hydraulic Properties
2.5 Sources and Sinks
2.6 Water Budget

3 Computer Code
3.1 Code Selection
3.2 Code Description

4 Groundwater Flow Model Construction
4.1 Model Grid
4.2 Hydraulic Parameters
4.3 Initial and Boundary Conditions
4.4 Selection of Calibration Targets

5 Testing and Calibration
5.1 Model Testing of geometric interpretations
5.2 Hydraulic Calibration and Residual Analysis
5.3 Hydraulic Sensitivity Analysis

6 Predictive Simulations

7 Summary and Conclusions
7.1 Model Assumptions and Limitations
7.2 Model Predictions
7.3 Recommendations

8 References
Appendices: Model Input Files

Figure 6-9. *Sample Table of Content of a groundwater flow model report. A modified reproduction of /ASTM, 1999/.*

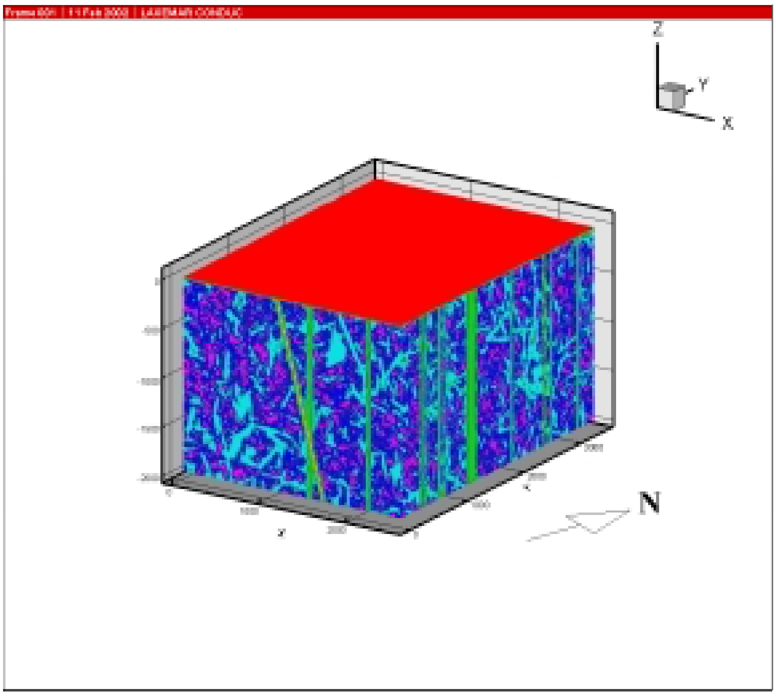


Figure 6-10. *3D visualisation of a hydraulic conductivity field in the Laxemar model domain /Andersson et al, 2002a/.*

If the model geometry is considered reasonable following the testing of the model by means of simulation, the groundwater flow model is calibrated. This means that properties as well as boundary conditions in the groundwater flow model will be adjusted to provide better correlation with observed entities such as piezometric levels, TDS distributions in boreholes and discharge areas. Interference tests are essential for the calibration. In Figure 6-11 an example is shown.

An important aspect is the comparison with hydrogeochemical data, especially TDS, see Figure 6-12. The hydrogeochemical understanding of the site can also be increased with help of flow paths calculated with the groundwater flow model using particle tracking. The flow paths are a critical for communication between the hydrogeology and hydrogeochemistry disciplines. Flow paths or the flow field within the modelled volume is an essential contribution from hydrogeology to hydrogeochemistry for their interpretation but also the hydrogeochemical interpretation of the chemical data and the flow field can both signal that something should be changed in the hydrogeological model as well as confirming consistency between the models and thus a greater reliability in the Site Descriptive model.

Recharge and discharge areas observed should also be reproduced by the groundwater flow model. In Figure 6-13 an example of the flow directions near surface illustrates the modelled recharge and discharge areas.

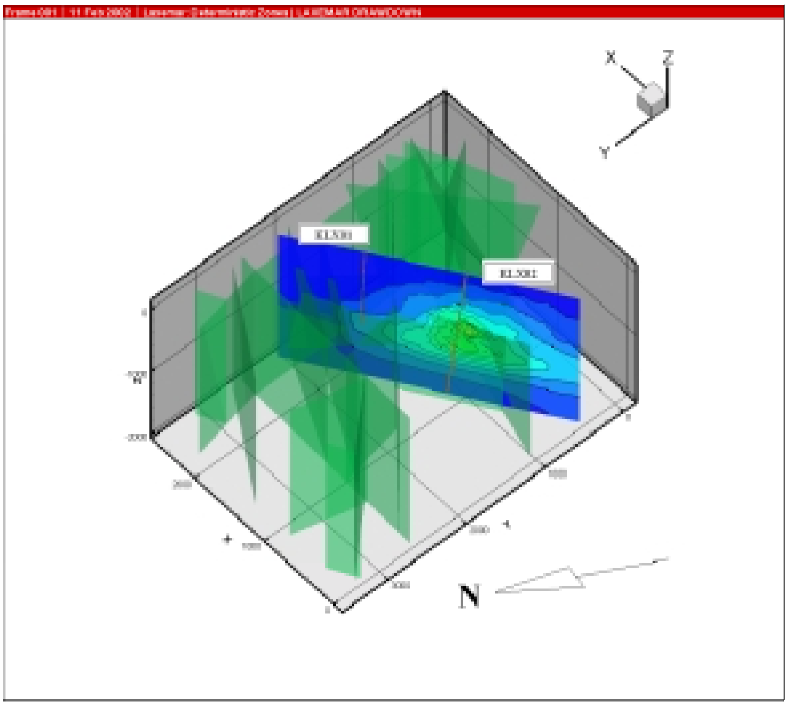


Figure 6-11. *3D visualisation of the drawdown in a vertical cross-section running through two boreholes in the Laxemar model domain /Andersson et al, 2002a/.*

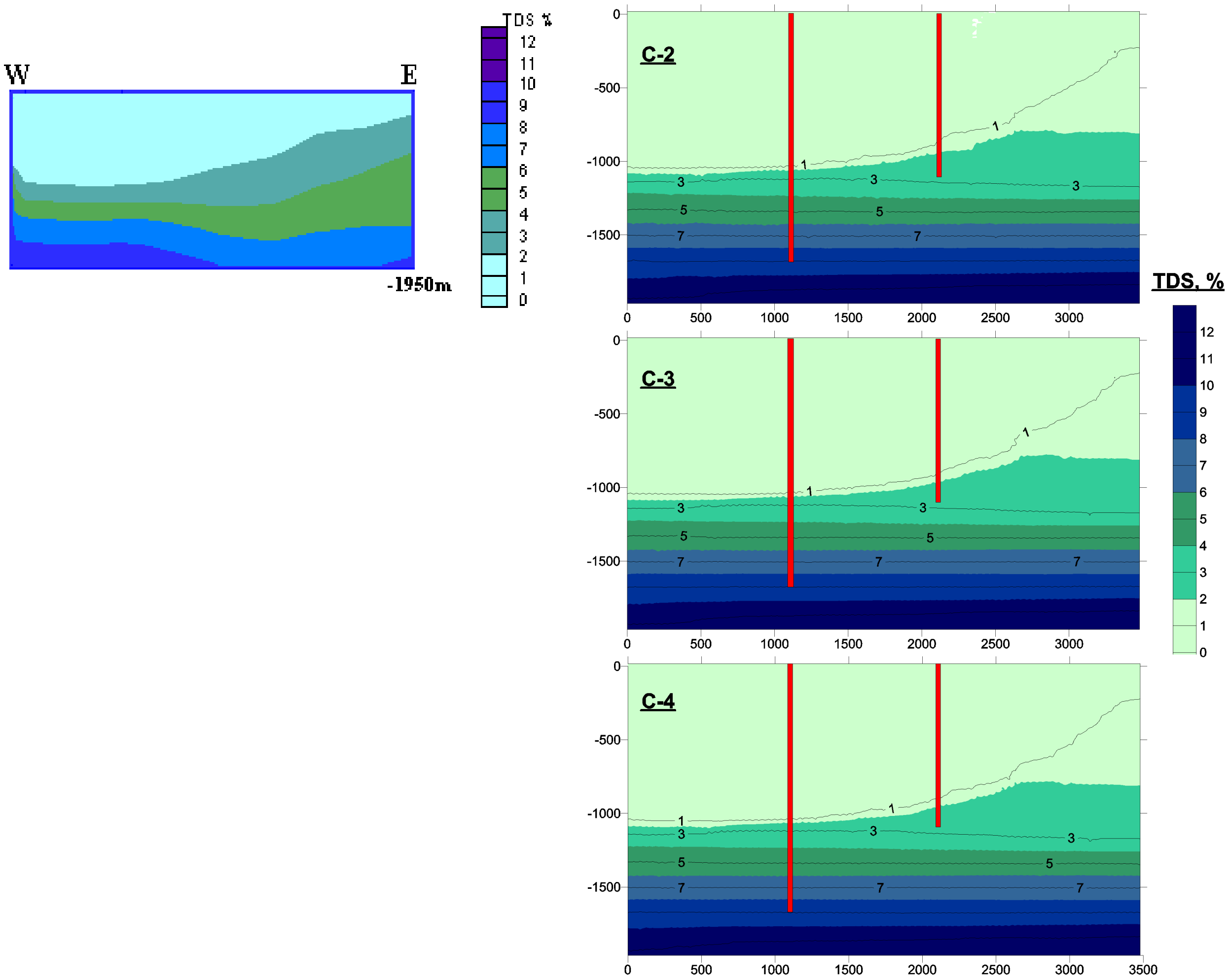


Figure 6-12. *Visualisation of TDS (in %) in a vertical cross-section running through two boreholes in the Laxemar model domain. Left: Interpolation between known and assumed values at a depth of –1950 m at the boundaries for the volume used for interpolation. Right: Simulation with a groundwater flow model, 3 realisations. /Andersson et al, 2002a/.*

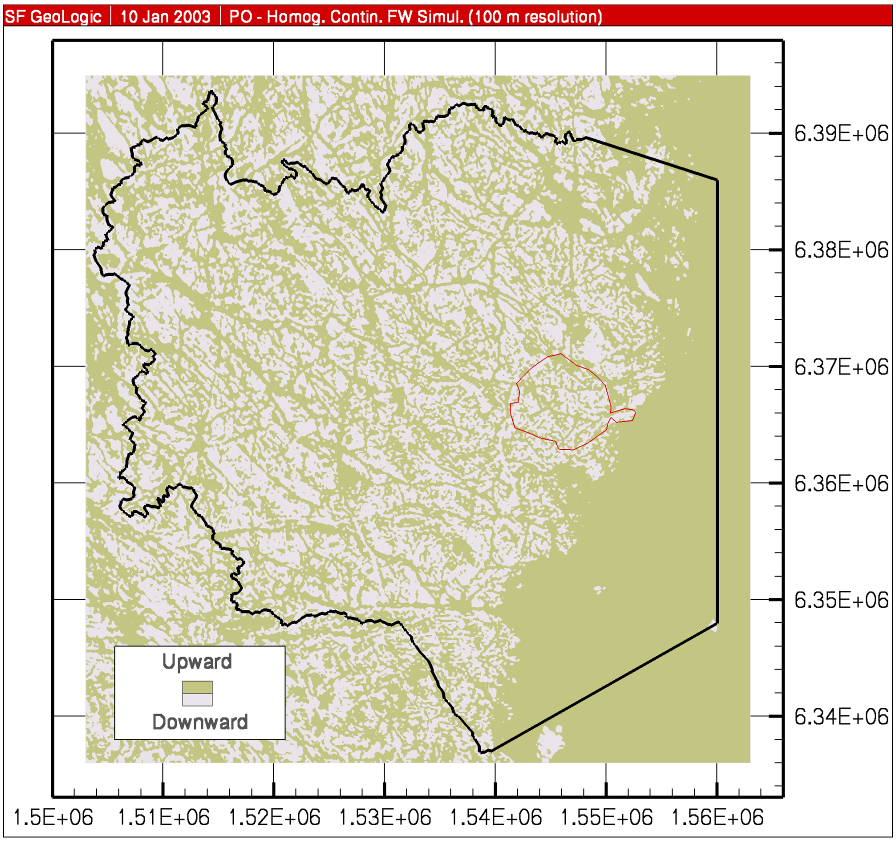


Figure 6-13. *Visualisation of flow directions near surface illustrating the modelled recharge and discharge areas. (Grid in meter) /Follin and Svensson, 2003/.*

6.5 Assessment of uncertainties and confidence in the Descriptive Model

The interpretation of domain geometry, hydraulic properties, boundary and initial conditions always includes uncertainties associated with measurement and data, spatial and temporal variability and conceptual issues. A general description of the assessment of uncertainties and confidence can be found in /Andersson, 2003/ and is also illustrated in Table 6-2.

There are several uncertainties associated with ***conceptual models***. It is essential for the investigations and the modelling that relevant processes have been identified, as the type of investigations as well as mathematical modelling and general conclusions made from the data depend on these processes.

Part of the conceptual model consists of ideas concerning the types of geometric elements to be identified. If these types of geometric elements turn out to be less relevant to the description, parameterisation and modelling of the site and possibly the type of investigations used will probably be of less value, thus confidence in the descriptive model will be eroded. In the same way, conceptual uncertainties also apply to a larger scale. The descriptive model may contain *alternative models*, which consist of:

Table 6-2. Uncertainties in Site Descriptive modelling.

	Conceptual models	Investigations	3D modelling, Calculations
Concepts	Incorrect process	Incorrect general assumptions	Incorrect mathematical model
Structures	Incorrect principal geometric description	Incorrect location	Incorrect implementation of domain geometry
Data	Incorrect parameter estimates: value (single measurement), variability and spatial distribution model	Measurement errors	Implemented properties, initial or boundary conditions incorrect

- An alternative geometric framework (i.e. deformation zone and rock domain geometry).
- Alternative descriptions within the same geometric framework (such as DFN or SC models or different parameter values or processes).

An alternative geometric framework implies a different geometry, such as new deformation zones, which were not included in the original model (for example including sub-horizontal zones as opposed to a base case with sub-vertical zones). When using *alternative descriptions within the same geometric framework* it is quite obvious that DFN and SC represent different concepts of parameter representation in space. What should also be considered, as an alternative model, is a totally different parameter representation within a DFN or SC model, e.g. constant value or stochastic distribution within HRDs in a SC model, linked to "data" in Table 6-2.

If the data provided for analysis have not expected measurement scale, or some type of data are lacking, it may be difficult to identify the spatial distribution model with its natural variability. This will cause uncertainties in the property assignment method. *Conceptual uncertainty* in the data can be difficult to quantify. At a parameter level, different interpretation methods are used, based on different conceptual models. By comparing pdfs based on different interpretation methods, the robustness of some parameters can be assessed. Hydraulic transient tests for example, can be evaluated assuming both stationary and transient conditions. Different hydraulic tests are performed for the same borehole sections, for example injection tests and PFL with 5 m measurement scale.

If the ***investigations*** are based on erroneous conceptual ideas, uncertainties in the model description may be great. Lack of site-specific knowledge may lead the investigator to focus on rock volumes that provide less information than if other rock volumes had been focused upon. The stepwise updating of models will make it possible to focus investigations on volumes where the site specific needs demand less uncertainty in the site description. Finally, the different kinds of measurements performed during the Site Investigations are all subject to measurement errors.

Measurement uncertainties (or measurement errors) can normally be quantified and may be random or systematic. There is always a random error in measurements due to the degree of accuracy of equipment and procedures. A systematic error may be due to erroneous calibration of instruments. Systematic measurement errors may be difficult to detect but a good Method Description and QC of collected data are aimed at reducing this uncertainty. The reporting of primary data includes a description of the measurement resolution and accuracy of recorded variables such as pressure and flow rate. These data can be used in conjunction with the interpretation models to estimate measurement uncertainty. Generally, measurement uncertainty can be considered insignificant.

The ***3D modelling*** of a site is also linked to the conceptual errors mentioned above. If essential processes are not known, it is obvious that they cannot be mathematically modelled. There are also uncertainties in the interpreted geometric model. A deformation zone, its position, extent and orientation as well as a rock domain contain uncertainties. In Figure 6-14 the uncertainty pertaining to the position of a deformation zone is captured by defining a *Modelled uncertainty of Deformation zone.* See /Munier et al, 2003/ for further details. This Modelled uncertainty is one tool for defining *alternative positions of specific deformation zones* that can be transferred from RVS to a groundwater flow model in order to test the implications of the different positions on the flow field. This uncertainty is referred to as *data uncertainty* and is not an "alternative geometric framework".

Finally, data will always represent some average value of a given volume (and/or over time). If the measurements are made at different points in space (or time) and are not constant (excluding the uncertainties in measurements), the variable has a spatial variability (or temporal variability). By means of measurements, Cumulative Distribution Functions (cpf) or Probability Density Functions (pdf) can be used to describe a variable. The spatial correlation can be analysed for a spatial sampled variable, and for a time-sampled variable the time correlation can be analysed. Uncertainties associated with variability in space or over time can be estimated from these statistical models. Different boundary conditions can be tested in numerical groundwater flow models to explore the effect on the flow field.

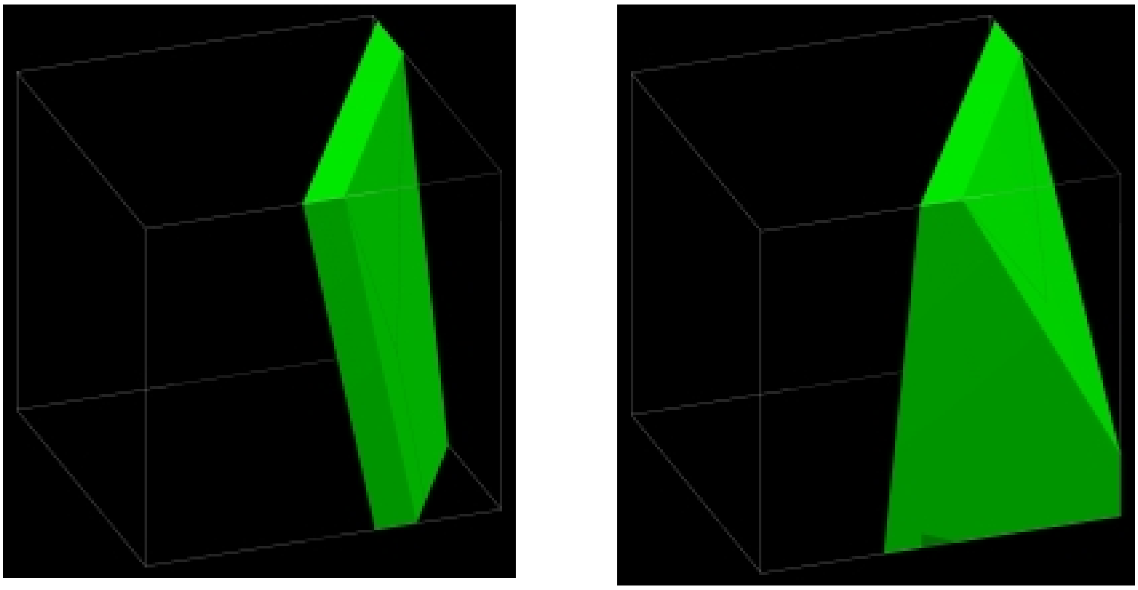


Figure 6-14. *Visualisation of Modelled Uncertainty of Deformation zone. Left: dip of structure is considered uncertain. Right: With data from a greater depth in the rock mass confirming the structure, the MVS becomes smaller /Munier et al, 2003/.*

The above 3D model data and structure uncertainties can be referred to as *data uncertainty*; the uncertainty in the parameter values of a model. It should be pointed out that, while the uncertainty of the *existence of a structure* may be small*,* the uncertainty of the *structure's property* (data) may be significant. It is easier to show the existence of a structure than to assess its properties precisely.

Groundwater flow models are useful for assessing uncertainty in the descriptive model, by first making a sensitivity analysis of a selected number of performance measures (e.g. piezometric levels and flow paths) for a specified geometric framework and its properties. Similar analyses of different alternative geometric frameworks with alternative models of parameter fields will provide the basis for an overall assessment of the uncertainty and confidence in the descriptive model.

The performance measures used should be able to show:

- to what extent new information modifies essential hydrogeological conditions,
- the robustness of the model, in terms of important modelling issues.

Useful performance measures in this context are able to:

- test the general flow pattern in the model that forms the base for the general understanding of the site,
- test transport related issues relevant to the safety of the repository,
- test groundwater issues related to the environmental impact of the construction of the deep repository.

The consistency checks made by comparing modelling results from the different disciplines provide yet another means for the description of confidence in the descriptive models. These consistency checks have been briefly mentioned in the previous chapters. Some consistency checks are outlined below:

- Interference tests are very useful for testing the geometric model of deformation zones and their connectivity. The limitation is that low transmissivity deformation zones cannot generally be tested and, as the investigated volume is large, the geometry and connection between all deformation zones cannot be tested. Interference tests in the soil (regolith) may also prove useful for testing the geologically defined geometry of boundaries as well as geological interpretation of the continuity and permeability of soil layers.
- Multiple-borehole tracer tests carried out by the Transport discipline are similar to interference tests for testing the geometric model of deformation zones and their connectivity. Dilution tests in observation sections also provide a more direct observation than pressure response, providing a significant flow and not just a "dead end".
- The spatial distribution of the actual (undisturbed) condition of TDS, the TDS changes in the pumped water during pumping tests and the current knowledge about the evolution of the Baltic sea since the last glaciation provide hydrogeochemical data that should agree with the groundwater flow modelling results (paleohydrogeological modelling and modelling of interference tests).

- Hydrogeochemical observations and modelling conclusions pertaining to chemical reactions and mixing should agree with the hydrogeochemistry of fracture minerals, organic material, redox conditions etc along the flow paths modelled.
- The modelled discharge areas should agree reasonably well with the mapped springs and wetlands as well as the probable discharge areas based on the Surface Ecosystem interpretation of the vegetation map.
- Rock mechanics stress modelling indicates stress magnitudes and stress ratios, which in turn may indicate the major directions of hydraulic anisotropy. Some observations in Sweden indicate that this coupling exists, although one could argue that chemical precipitation in the open fractures will over time decrease the anisotropy induced by a stress field that is millions of years old. Daily dynamic stress changes caused by the earth-tides may be the reason why this anisotropy appears to exist.
- Permeability changes with depth may be related to changes in fracture intensity and/or stress.

6.6 Reporting of Descriptive Model

6.6.1 Site description

If the X.Y version model and its alternatives are considered relevant in relation to the available data, the model geometries, properties and boundary conditions should be described in a systematic and condensed way. The properties of the domains reported are both those suggested from the analyses of the tests and the calibrated groundwater flow model of the alternatives modelled.

In the descriptive model, the reported parameters cover both the regional and the local scale. Tables 6-3 to 6-7 indicate how some of the parameters may be reported for a model alternative. If no site-specific data are available for a parameter, data from other SKB investigations or general scientific information is used for the first estimate.

Table 6-3. Base Hydrogeological Model. Suggested transmissivity for Hydraulic Conductor Domains (HCD). "Other zones" are based on expert judgment and the mean transmissivity of the zone within the Regional Site Descriptive model.

Zone name	Transmissivity (T) (m^2/s)	Estimated possible range for T (m^2/s)	Comment
ZLXNE03	7×10^{-6}	0.1T<T< 10T	
ZLXNE04	7×10^{-6}	0.1T<T< 10T	
ZLXEW01	1×10^{-4}	0.1T<T< 10T	Regional zone
ZLXNE01	1×10^{-4}	0.1T<T< 10T	Regional zone
Other zones	3×10^{-6}	0.1T<T< 10T	Local zones

Table 6-4. The power law relationship between transmissivity (T) and Storage coefficient (S). Test scale approximately 100 m. S = aT^b. R=Correlation coefficient. n = sample size /Rhén et al, 1997c/.

Scale (m)	a	b	R	n
100	0.009	0.79	0.71	5

Table 6-5. Lognormal distributions based on univariate statistics for KLX01 and KLX02, with zones in Table 6-3 excluded from the data set for analysis. Data represent measurements along sub-vertical boreholes.

HRD	Description scale (m)	Hydraulic conductivity (K)	
		Median(Log10(K)) (m/s)	Std(Log10(K)) (m/s)
HRD1	5	–10.5	1.8
	20	–9.0	1.4
	100	–7.4	1.1
HRD2	5	xxx	xxx

Table 6-6. Geometric and hydraulic properties of the non-deterministic fractures in HRD1.

Set	Orientation statistics of the mean normal vector (pole)				Fracture size	Spatial distribution	Fracture intensity	
No.	Type	Trend	Plunge	Dispersion	D	Type	P_{32}	P_{32c}
1	Fisher	262.0	3.8	8.52	–2.6	Baecher	0.78	0.12
2	Fisher	195.9	13.7	9.26	–2.6	Baecher	0.66	0.15
3	Fisher	135.9	7.9	9.36	–2.6	Baecher	0.76	0.12
4	Fisher	35.4	71.4	7.02	–2.6	Baecher	0.24	0.08
All	$T \in logN(4.2 \cdot 10^{-8}, 2 \cdot 10^{-7})$ m^2/s [$\approx log_{10}T \in N(-8.06, 0{,}773)$ log_{10}(m^2/s)]						2.44	0.48

Given the value of the Power Law Exponent, *D*, and the volume, *V*, of the Laxemar model domain, the number of fractures (squares in DarcyTools), $N[L_1, L_2]$ within a specified size range, L_1 to L_2, can be estimated using the following equation (taken from /Andersson et al, 2002a/):

$$N[L_1, L_2] = \frac{V\,I}{D}\left[\left(\frac{L_2}{L_{ref}}\right)^D - \left(\frac{L_1}{L_{ref}}\right)^D\right] \qquad (6\text{-}1)$$

where $L_1 < L_2$. *I* and L_{ref} are two coefficients that determine the position of the power law distribution in a log-log plot of *N* versus *L*. For the structural-hydraulic model of the Laxemar model domain, the following coefficients are used: $D = -2.6$, $L_{ref} = 500$ m and $I = 10^{-8}$.
A positive correlation between the size of the hydraulic features and the transmissivity (T_f) is assumed:

$$T_f = \begin{cases} \alpha \left(\dfrac{L_f}{100}\right)^2 \ \mathrm{m^2/s} \quad \text{for } L_f \leq 100\,\mathrm{m} \\ \alpha \qquad\qquad \mathrm{m^2/s} \quad \text{for } Lf > 100\,\mathrm{m} \end{cases} \qquad (6\text{-}2a)$$

$$b = 0.01\,L_f \qquad (6\text{-}2b)$$

The value of the coefficient α in Equation (2a) was set *at* 10^{-8} $\mathrm{m^2/s}$ (taken from /Andersson et al, 2002a/).

Table 6-7. Typical ranges for HSD hydraulic properties (No measurements available for this model version) /Carlsson and Gustafson, 1997).

Soil type	Hydraulic conductivity (m/s)
Till	$10^{-5} – 10^{-11}$
Clay	$10^{-8} – 10^{-12}$
Silty soil	$10^{-5} – 10^{-9}$
Sandy soil	$10^{-3} – 10^{-6}$

6.6.2 Numerical groundwater flow simulations for understanding and description

The groundwater flow modelling for each site is reported in a separate report, including results from different computer codes used. These reports detail the concepts and mathematical formulations, spatial assignment methods, initial and boundary conditions, calibration, conditioning and the simulations required for a general understanding of the site.

A summary of concepts, calibrations etc and important results are included in the report on the descriptive model. Important results are illustrations of pressure and salinity distribution in the bedrock and soil deposits as well as of flow paths and discharge areas under natural conditions.

6.6.3 Overall assessments of uncertainties and confidence of the descriptive model

The assessments of uncertainties of and confidence in the model’s geometric frame work and assigned properties are discussed and summarized. See /Andersson, 2003/ for further details. The need for further refinements and a decrease in uncertainties is discussed in respect of future requirements for a general understanding of the site, Design of the deep repository and Safety Assessment.

6.6.4 Suggestions for new investigations

Based on the overall assessment of uncertainties and confidence in the descriptive model, volumes of rock and soil can be identified where new investigations would reduce the assessed uncertainties. Suggestions are made regarding the type of investigations and where they should be performed.

6.7 Numerical groundwater flow simulations: Planning of field investigations and exploratory simulations

6.7.1 Objective

The general idea behind exploratory simulations is to benefit from the formalised modelling procedure described in Section 6.4 and Figures 1-2 and 6-6. By using only certified (established) model versions the outcome of exploratory simulations is expected to be of practical use for decisions relating to the questions studied.

6.7.2 Certified model versions

The first certified version of the Site Descriptive Hydrogeological Model that has also been implemented in a numerical flow model is version 1.1. Version 1.1 (or v1.1), will be followed by at least three other model versions, namely v1.2, v2.1 and v2.2. The differences between the model versions are described in Table 1-1. In brief, as more information is gathered about the physical hydrogeological system, the more comprehensive is the numerical flow model. In this respect, versions 1.2 and 2.2 are more elaborated flow models than v1.1 and v2.1. According to Table 1-1, v1.2 is intended to support the Preliminary Site Description and v2.2 (or subsequent versions) the Site Description. This means that v1.2 and v2.2 (or subsequent versions) are also the required flow model versions for support of the corresponding mandatory design calculations and safety assessment simulations.

6.7.3 Examples of applications of exploratory simulations

Unlike the modelling procedure behind the certified model versions, exploratory simulations are intended to focus on specific questions. The questions may be raised by any of the principal activities; *investigations*, *design* and *safety assessment*. The questions may also be raised by the *coordinate function* responsible for the overall evaluation of the sites and coordination between different principal activities and different sites.

Questions of specific interest for *investigations* are typically those dealing with the planning of forthcoming field activities, for example:

- What is the most appropriate design for a multi-packer monitoring system in a given borehole in relation to a planned interference test or tracer test?
- What is the expected hydraulic response of a planned interference test at a location not currently investigated by means of drilling?

Questions of specific interest for design are typically those dealing with the planning of the repository layout, for example:

- What are the predicted water inflows to shafts, ramps, deposition drifts and canister holes in alternative repository layouts?
- What is the water table drawdown and what is the saline groundwater upconing in alternative repository layouts and construction methods?

Questions of specific interest for safety assessment are typically those dealing with the reported field results and the layouts considered, for example:

- What are the advective travel times between a proposed repository layout and the biosphere with or without consideration of the variable density effects (saline groundwater)?
- What are the Darcy fluxes at repository depth under pre-disturbed and post-disturbed groundwater conditions?
- What are the transport resistances (F-factors) of the fracture network for flow paths from the deep repository?

The above questions are just a few examples of the wide range of questions that may be raised. In keeping with the modelling procedure behind the certified model versions, exploratory simulations should be specified by a Task Description (cf Secton 6.4), which lists SKB’s general and specific objectives for exploratory simulations and specifies a minimum level of quality assurance in the model setup and expected output.

7 Information and documentation management

Investigations, interpretations and 3D modelling all generate data that are reported in written and/or digital format as described in Figure 1-2. In this chapter an overview of information and documentation is given.

7.1 Primary data

Field investigations and the inventory of available information are controlled by Activity Plans that generally consist of Method Descriptions, Instructions and Routines. These documents detail the general performance of the field investigations (Company, personnel, where, when, how), QC, written report, digital delivery of measurements and interpreted parameters. Templates are provided for the written report and the interpreted hydraulic test parameters.

All data collected during field investigations are called "Primary data". Primary data consist of "Raw data" and "Routine work up and calculated data". Raw data in digital format are stored in SICADA (Site Characterisation Database) or the GIS database SDE (Spatial Data Engine) and other material in the Field Archive. The Routine work up and calculated data are the data interpreted based on a standard procedure. The interpreted parameters from a field investigation are digitally delivered to the SICADA database and presented in a written report. The written report also includes a description of the field investigations, QC etc. Details about the performance of the investigations and QC are documented in protocols that are stored in the Field archive and in an activity log in the SICADA database.

The monitoring of piezometric levels, levels in watercourses, lakes and the sea, meteorological data and flow rates in watercourses are generally stored on a continual basis at a database at SKB. Most data are stored in the HMS (Hydro Monitoring System) database. Some monitoring may take place with freestanding data loggers. The data are then collected on a routine basis from the data logger and stored in the HMS database at SKB. Data such as the daily values of piezometric levels can also be transferred to SICADA.

7.2 Analysis of Primary data

The analysis of Primary data is based on data from the SICADA and SDE databases as well as written reports. If it is necessary to check the performance of a particular investigation, the Field archive will be used.

Reported parameter values are examined to detect extreme values. If the extreme values detected are found to be typing errors or misinterpretation, the values in the database are amended.

Some hydraulic tests may lack some information on fluid properties. Information from other sources, mostly geophysical logging and analysed water samples, is used to complement the SICADA database.

Grain size distribution curves are used to calculate hydraulic conductivity for samples during drilling or digging in the surficial deposits. These data are stored in the SICADA database.

Hydrological data (Meteorology, run-off, levels in lakes and the sea) are compiled and analysed. Interpretation of surface water divides (and possibly groundwater divides) is updated if necessary and stored in the GIS database.

An overview of primary data is prepared with WellCad and preliminary univariate statistics are composed, although this information is merely stored locally for the project group engaged in producing the descriptive model. Other data are also compiled and stored locally.

7.3 Integrated evaluation and Site description

The integrated evaluation is performed in steps and the geometric framework, domain properties and boundary conditions are updated. In this process, data are stored locally for the project group involved in the development of the descriptive model.

When the X.Y. version model and its alternatives are considered relevant in relation to the data available, it is stored as an official model version in the RVS and SDE databases. The X.Y version model is also reported on in a written format, including an overview of data collected, a summary of the evaluation of primary data, a summary of the 3D integrated modelling, an overall assessment of uncertainty and confidence pertaining to the model and finally; a condensed description of the X.Y version model. All disciplines report their descriptions in the same, integrated, report.

The geometric information concerning deformation zones, rock units and boreholes is imported from RVS, where the geology discipline updates deformation zones and rock unit information during the integrated evaluation. The Hydrogeology discipline can work with the RVS and produce “Hydrogeology-versions” of the model in RVS for discussion within the project group. The official X.Y version model in RVS contains the HCDs and HRDs and possibly the HSDs. The properties and boundary conditions are described in the written report but some data may be stored in the SICADA and SDE databases as X.Y version model data.

8 Updating of this report

This report describes the process of developing a hydrogeological site descriptive model. It provides a structure for the work but some details have to be developed during the actual modelling. The modelling is considered to be a learning process, and therefore the modelling strategy must be flexible and updated as required.

This document is intended to guide the modelling at the different sites with the aim of achieving consistent handling of modelling issues during Site investigations. Based on the experience gained from the Site Investigations, the project teams involved in the integrated modelling of each site can make suggestions for the updating of the report. SKB will update the report as required.

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Appendix 1

Overview of Method Descriptions relevant to Hydrogeology

Table A1-1. Compilation of main Method Descriptions (MD) guiding the data collection for the interpretation of hydraulic properties and boundary conditions.

MD	Method	Method specific interpretation	Co-interpretation
390.001	Borehole inventory and construction data for hydrogeological documentation of the area.	Inventory of hydrogeological data may result in a wide spectrum of data from domestic wells, groundwater handling facilities, drainage projects, hydrogeological data from constructed facilities, land use, vegetation etc. Some of these data are compiled during the feasability studies.	Co-interpretation will be made with similar data collected during the site investigation.
364.007	Meteorological measurements.	Meteorological measurement station(s) will be built if there are no suitable stations in or near the investigation area. Measurements consist of; air temperature, air pressure, precipitation, relative humidity, global radiation, wind direction and wind speed. Potential evapotranspiration is calculated from these data.	Co-interpretation may be made with data from near-by meteorological measurement station(s) with longer recorded time series.
364.008	Surface hydrological measurements.	Runoff rates and water levels will be measured in a few water courses. The catchment area is estimated and specific runoff is calculated for stations where runoff rates are measured.	Co-interpretation may be made with data from near-by meteorological measurement station(s) with longer recorded time series.
364.009	Oceanografic measurements.	Water level, water temperature, salinity, current speed and direction turbidity, sea water transparency, duration of ice formation and breaking up of ice will be measured at one or more measurement stations. All parameters may not be measured at all stations. Water level and salinity are of primary interest for hydrogeology.	Co-interpretation may be made with data from near-by meteorological measurement station(s) with longer recorded time series.

131.001	Overburden characterisation method description.	The description covers several types of method for characterising soil (regolith) deposits. Of special interest for hydrogeology is grain-size curves and interpreted stratification.	
610.003	Percussion drilling.	The description covers several types of percussion drilling and the methods used to collect data during drilling. Of special interest for hydrogeology are the drilling rate and the surface measured flow rate.	BIPS (Image of the borehole wall) is used to detect lager fractures and rock types.
620.003	Core drilling method description.	The description covers several types of core drilling and the measures taken to obtain continuous cores and an open borehole for further investigations. The mapped open natural fractures are of special interest for hydrogeology.	BIPS (Image of the borehole wall) is used for core mapping and is vital in terms of the orientation of the core.
630.003	Overburden drilling method description.	The description covers several types of overburden drilling. It describes the measurements and samples taken during drilling as well as the installation of observation wells. Of special interest for hydrogeology are the grain-size distribution curves from samples of various depths to the bed rock.	Drilling provides information about the soil (regolith) deposits for the geological descriptive model. Results from hydraulic tests in observation holes are a part of the co-interpretation.
640.001	Method description for the registration of drilling parameters and sampling of drilling water as well as drill-cuttings during core drilling.	Drilling water is monitored to establish a basis for the waterbalance and total drillwater volume calulations as well as a control to ensure that the injected drillwater is oxygen free. Weighing of drill-cuttings during core drilling provides a base for the estimation of how much of the drill-cuttings have intruded into the fractures.	Co-interpretation will be made with the preliminary coremapping and drilling parameters to indicate sections where water samples should be taken during drilling with the wireline equipment presented in MD 321.002.

321.002	Pump test, pressure measurement and water sampling in connection with wireline drilling.	Wireline drilling can be interrupted and water samples can be taken from a test section below an inflated packer. The pressure in the test section and the flow rate during pumping can be measured to obtain hydraulic properties. Only pressure measurements can be made to provide the undistrurbed pressure of the test section.	Co-interpretation will be made with the preliminary core mapping. The results will be compared with the results from other hydraulic tests performed after the drilling is completed.
225.004	Instructions for length calibration.	All measurement tools used in the coreholes must be length calibrated to ensure optimal accuracy of every measurement made in the core-hole. Length marks made during drilling in the borehole wall serve as a point of reference.	In all co-interpretation of corehole data, the correct length must be ensured.
322.009	Flowlogging-Impeller.	The borehole is flow logged with an impeller probe to obtain the cummulative flow rate along the borehole during pumping with constant drawdown. The probe can also measure temperature and electrical conductivity. The pumping before the logging together with the subesquent recovery is treated as a pump test of the entire borehole and is used in conjunction with flow logging data to estimate the transmissivity distribution along the borehole. It is used as a complement to PFL-Diff, as the latter has a limited upper measurement range.	The anomalies are compared with the core mapping.

322.010	Difference Flow Logging Methodology.	With the Posiva Flow Log – Difference Flow logging method (PFL-Diff), the flowrate can be measured in a test section during natural (undisturbed) conditions as well as during pumping of the borehole. If two drawdowns are used, transmissivity and the undisturbed pressure of the measurement section can be estimated. If the measurement section is moved in small steps it is possible to detect the position of more conductive fractures. Several logging modes are used to estimate the natural groundwater flow, transmissivity and undisturbed pressure along the borehole in a defined test section length L_w indicating the positions of individual conductive fractures using step length dL. The probe can also measure single-point resistance, elctrical conductivity and temperature. Logging of absolute pressure (high resolution pressure transducer) or Freshwater head measurements (measured with a hose) are also carried out.	BIPS and core mapping are used to identify hydraulic features. The transmissivty and orientation of individual fractures established to some extent.
325.001	Slug test method description.	Slug tests are made in boreholes, mainly in soil (regolith) deposits in order to estimate the hydraulic conductivity of (a part of) the deposits or to control the function of the borehole as an observation section for pressure responses.	The geological interpretation of the seqence of soil (regolith) deposits penetrated by the borehole as well as results from the sieving of samples taken during drilling.

323.001	Hydraulic injection test method description.	The injection test is performed in a limited part of the borehole using packers. Tests are performed as constant pressure tests with an injection and recovery phase and hydraulic properties of the measurement section are interpreted (generally transmissivity, skin and wellbore storage, depending on the hydraulic conditions). At the surface the temperature and electrical conductivity of the pumped water is measured if the SKB (PSS or HTHB) equipment is used.	BIPS and core mapping are used to identify hydraulic features. Results are also compared to flowlogging results.
321.003	Hydraulic single-hole pumping test method description.	Pumping tests are performed in an open borehole (testing the entire borehole) or a limited part of the borehole using packers. Tests are performed as constant rate tests with a pumping and recovery phase and hydraulic properties of the measurement section are interpreted (generally transmissivity, skin and wellbore storage, depending on the hydraulic conditions). At surface the temperature and electrical conductivity of the pumped water are measured if the SKB (PSS or HTHB) equipment is used.	BIPS and core mapping are used to identify hydraulic features. Results are also compared to flow logging results.
330.003	Interference test method description.	The borehole section is pumped and analysed in a similar way as for Single-hole pumping tests. Drawdown and recovery responses in observation sections are primarily used to analyse connectivity between the interpreted HCDs. Response times and final drawdown are primary data for interpretation. Depending on geometric and boundary conditions, it may be possible to interpret the storage coefficient for some HCD and local boundary conditions.	The geological 3D deformation zone model is used for the first analysis. As a second step, interference tests are used to test a 3D groundwater flow model.

320.004	Instructions for analysis of injection and single-hole pumping tests.	Analysis of hydraulic tests presented in MD 321.002, 322.009, 322.0010, 323.001, 323.002, 321.003 and 330.003 should be made in a similar way. In this MD, general requirments are presented for analysis and reporting.	The current geological descriptive model forms a base for an understanding of the interpretation.
530.006	Method description for multiple-borehole tracer tests.	The borehole section is pumped and analysed in a similar way as for Single-hole pumping tests. The results can resolve some large scale connectivity issues and (fairly) local transport properties. The method is described in /Berglund et al, 2003/.	The geological 3D deformation zone model is important, as it forms a base for the analysis and co-interpretation between geology, hydrogeology and transport. As one tool, multiple-borehole tracer tests are used to test a 3D groundwater flow model.
350.001	Borehole dilution test method description	A dilution test is performed in a borehole section to estimate the groundwater flow through that particular section under natural (undisturbed conditions) or during a pumping test. Data are useful for assessing local hydraulic connectivity and estimating the range of the groundwaterflow in the rock (or soil (regolith) deposit). The method is described in /Berglund et al, 2003/.	The co-interpretation between geology, hydrogeology and transport is important for general conclusions about the dilution measurements.

Appendix 2

3D groundwater flow modelling codes

Continuum code (DFN- based) – DarcyTools

The specified geometries and hydraulic properties of the deterministic and random hydraulic features are implemented into DarcyTools, which is a volume-integrated finite-difference code for variable-density groundwater flow.

DarcyTools uses a mixed DFN/Continuum approach for the simulation of groundwater flow through fractured rocks. That is, the geometries and the transmissivities of all discrete features are transformed into equivalent inter-node conductivities prior to the solution of the flow equations. Hence, DarcyTools models flow through an anisotropic and heterogeneous continuum. The modelling technique is described in detail by /Svensson, 2002a,b/.

Nammu and Connect flow

NAMMU is a computer program for modelling groundwater flow and transport through porous media. Temperature as well as the transport of solutes can be modelled. Density dependent flow and Unsaturated conditions can also be modelled. Details about the code can be found in /Cliffe et al, 1999/.

CONNECTFLOW (CONtinuum and NEtwork Contaminant Transport and FLOW) is a software package for modelling groundwater flow and transport in porous and fractured media. It is based on the NAMMU and NAPSAC software and provides all of the functionality of NAMMU and NAPSAC. In addition, it enables combined models to be built consisting of NAMMU (porous medium) and NAPSAC (fractured rock) sub-models. This allows the most appropriate models to be used. It incorporates full 3D grid generation and post-processing capabilities. Details can be found in /CONNECTFLOW, 2002/.

DFN code – Fracman/Mafic

The conceptual model used in the Discrete Fracture Network approach assumes that discrete fractures provide the primary hydraulic flow paths and connections, and that accurate representation of flow path geometry is a key to successful hydrogeological analysis. The fracture nenetwork is modelled by the FracMan program package by Golder Associates, Inc /FracMan, 1996/.

When the DFN model is properly "calibrated", the hydraulic behaviour of the model is calculated by the MAFIC program. MAFIC (Matrix/Fracture Interaction Code) is a finite element program used to simulate transient flow and solute transport through three-dimensional rock masses. MAFIC handles all types of network geometry and objects modelled by FracMan such as tunnels, deterministic objects, deposition holes etc.

The principle of DFN modelling is based on Monte Carlo simulations. This means that the hydraulic behaviour of a fracture network is modelled by several stochastic realisations (fracture networks) with the same stochastic parameters. The confidence in the hydraulic behaviour of a fracture network is built on the statistical analysis of the results of the multiple realisations.