TECHNICAL REPORT

98-02

Parameters of importance to determine during geoscientific site investigation

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June 1998

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PARAMETERS OF IMPORTANCE TO DETERMINE DURING GEOSCIENTIFIC SITE INVESTIGATION

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Information on SKB technical reports from1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26), 1981 (TR 81-17), 1982 (TR 82-28), 1983 (TR 83-77), 1984 (TR 85-01), 1985 (TR 85-20), 1986 (TR 86-31), 1987 (TR 87-33), 1988 (TR 88-32), 1989 (TR 89-40), 1990 (TR 90-46), 1991 (TR 91-64), 1992 (TR 92-46), 1993 (TR 93-34), 1994 (TR 94-33), 1995 (TR 95-37) and 1996 (TR 96-25) is available through SKB.

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Foreword

A fundamental prerequisite in SKB's work to site, build and commission a deep repository for radioactive waste is the long-term safety of the repository. This safety is based on the properties of the spent fuel, the performance of the engineered barriers and the properties of the bedrock. The importance of the geological conditions on the site for the long-term performance and radiological safety of the deep repository are analyzed and assessed in several stages. In the initial siting work, general siting studies and feasibility studies, general assessments are made concerning the fundamental preconditions for a deep repository. This is followed by site investigations, which are supposed to lead to a preliminary confirmation of whether a site is suitable, and a preliminary adaptation of the layout of the deep repository to the properties of the rock on the site. The final evaluation of the safety of the deep repository in its entirety is made during detailed characterization and repository construction. During these stages the detailed configuration of the repository is adapted to the actual conditions found to exist in the bedrock.

Before SKB commences site investigations (on at least two sites), an investigation programme will be presented that describes how the investigations are to be conducted and how the results will be used in evaluating sites. Here is meant above all the geoscientific investigations, since they will dominate during this siting phase.

The present report deals with the importance of geoscientific information for a deep repository. The intention is to structure in a pedagogical manner what kind of importance geoscientific properties and conditions have for the safety performance of the deep repository, for planning and design of the rock works, and for a fundamental geoscientific understanding of the site. The report serves as a basis for planning of the geoscientific investigations, which will progressively evaluate and define the siting and layout of the deep repository. For the site investigations in particular, the report comprises an important basis for the ongoing programme formulation work.

The contents of the report are based primarily on already identified parameter needs and widely accepted judgements regarding the importance of the information for the deep repository. In some cases, the evaluations made may be of a more subjective nature. As SKB gathers new information within the field, portions of the report will also be subjected to revision or refinement. This does not, however, lessen the importance of the report as a basis for the planning of geoscientific investigations.

Summary

This document identifies and describes geoscientific parameters that are of importance to know in order to be able to carry out performance and safety assessments of a deep repository for spent nuclear fuel, based on the information that can be obtained from a site investigation. The document also discusses data needs for planning and design of the rock works and for description of other environmental aspects. This information – together with a planned description of measurement, interpretation and analysis methods – comprises an essential body of background material for the geoscientific site investigation programme.

Another intention is that this document can be utilized to define with greater precision the acceptance criteria against which a site is evaluated. It is thereby verified that the parameters identified in this document include the so-called "siting factors" defined in the supplement to RD&D Programme 92 (SKB, 1994), even though certain parameters are reformulated, described in greater detail, or new. The document further attempts to provide a more detailed description of how different parameters influence safety performance, and how they are actually evaluated.

Finally, a supplementary goal is to clarify the information processing that takes place with data so that they can be utilized in the evaluation of a site's suitability. This clarification has been necessary to arrive at meaningful parameters, but should also be able to provide guidance in the planning of a future site evaluation. A planning of information processing is needed not least because it provides a basis for dividing the work into stages and for drawing up meaningful timetables for the geoscientific investigation programme.

To a large extent, the work has involved documenting and compiling *already identified* parameter needs, information channels and information processing routines within the disciplines of *geology*, *rock mechanics*, *thermal properties*, *hydrogeology*, *geochemistry and transport properties*. This document seeks to:

- clarify which parameters are of central importance in models for performance and safety assessment as well as other evaluation, and clarify how these parameters are derived from a geoscientific model description,
- identify which geoscientific parameters are needed to build a model that can deliver information of the above kind,
- discuss how the identified parameters are used, what importance they have, what precision is required (or can reasonably be expected) and which site-specific measurements may be utilized to determine the parameters.

The purpose of a geological model is to describe, as realistically as is possible (or necessary), the soil cover and the properties of the rock mass within a given area.

As a rule, the geological model is not used directly for the safety assessment, but primarily as a source of input data for the rock-mechanical, hydrogeological and geochemical models. The geological model also comprises the basis for the geoscientific understanding of a site. The geological parameters that are needed for the geological model can be divided into topography, soil type description, lithology and structural geology.

The evaluation of mechanical stability includes analysis of long-term mechanical stability for the repository's tunnels and sensitivity to large-scale changes in the load situation (e.g. a glaciation), evaluation of stability in the near field, both during operation and in the long term, coupled with analysis of a suitable configuration of deposition tunnels and deposition holes, an evaluation of stability under dynamic loading (e.g. earthquake), long-term mechanical impact on groundwater flow (mainly in the near field) and construction analysis. The rock-mechanical information can be divided into geometry of discontinuities, mechanical properties of fractures, mechanical properties of intact rock, mechanical properties of rock mass, density and thermal data, plus boundary conditions and supporting data.

Temperature and temperature distribution are fundamental condition parameters in the deep repository and have a direct influence on repository layout. The temperature influences the mechanical environment, groundwater flow and the chemical/biological environment, even though the influence is relatively moderate within the temperature range normally considered to prevail in the deep repository. Temperature parameters include thermal properties of the rock and temperatures.

Hydrogeological models have several areas of application in safety assessment and activities supporting safety assessment. A hydrogeological understanding also needs to be built up to explain long-term geochemical changes and coupled hydraulic and rock-mechanical phenomena. These applications are tied to different scales, and the need for input data differs slightly for these needs. In brief, models are used (or can be used) for hydrogeological understanding, boundary conditions for detailed models, predictions of large-scale changes in groundwater chemistry etc., predictions of inflow during the construction period, and resaturation after closure, input data to migration models, input data (flow) to near-field models (near-field flows), input data to biosphere models, and evaluation of (other) near-surface environmental consequences (land and environment). Hydrogeological parameters include geometry, permeability distribution etc. for both deterministically and stochastically represented discontinuities, hydraulic properties of the groundwater, hydraulic properties of the soil layers, and boundary conditions and supporting data.

The description of the water chemistry on the site and at the depth being considered for the repository is an important part of a safety assessment. The water composition is then used to evaluate different processes of importance for safety or as direct input data to calculations, for example the calculations of solubility and speciation of radionuclides that are usually included in a safety assessment. The water composition that is used to make such assessments does not, however, have to be completely identical to the groundwater chemistry that has been measured. A geochemical model which is capable of describing the chemical composition of the groundwater in different parts of the rock and how this chemical composition will develop needs to be set up. In summary, groundwater chemistry is of importance for assessing canister corrosion, bentonite performance, fuel dissolution and solubilities, radionuclide retention, and for a geoscientific understanding. Different parts of the groundwater composition are of different importance for these phenomena.

The transport models used in the safety assessment obtain their data to a large extent from the geoscientific description of hydrogeology and geochemistry. The model concepts are often directly adapted to a safety assessment point of view where actual, but difficult-to-characterize, mechanisms are simplified in a conservative direction. It can therefore be discussed whether nuclide transport models constitute a part of, or are rather based on, the geoscientific description. On the other hand, transport modelling makes new demands on site-specific data that are not automatically satisfied by the hydrogeological or geochemical description. The data requirement for transport modelling includes properties on a near-field scale, properties for flow paths (e.g. Darcy flow and flow-wetted surface), properties along flow paths (e.g. matrix diffusivity, sorption), properties of the soil layers and supporting data (such as tracer tests and groundwater-chemical analyses).

Finally, it is observed that the present document can serve as a point of departure for:

- a description of measurement, interpretation and analysis methods,
- a description of how data are analyzed in safety and performance assessments and the need for feedback to the site investigation programme,
- a discussion of more precisely defined site selection factors,
- a discussion of in what logical sequence different measurements need to be carried out with regard to both the need for input data and influence on other measurements.

Together, this information should comprise an essential body of background material for the planning of a geoscientific site investigation programme. It should also be pointed out that the present document needs to be constantly revised and updated, for example based on experience from the on-going safety assessment study SR 97. This notwithstanding, it may also be used in its current form for the necessary planning.

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1 Introduction

This document identifies and describes geoscientific parameters that are of importance to know in order to be able to carry out performance and safety assessments of a deep repository for spent nuclear fuel, based on the information that can be obtained from a site investigation. The document also discusses data needs for planning and design of the rock works and for description of other environmental aspects. Evaluation of the different parameters is discussed in the document as well. The document was produced by a working group consisting of the authors and various SKB staff and consultants, and comprises a step in the planning of a geoscientific investigation programme at the sites where site investigations will be conducted.

1.1 Purpose and strategy

1.1.1 Purpose

The goals of the work presented in this report can be derived directly from SKB's ongoing RD&D Programme (RD&D-95, SKB, 1995a). The latter programme stipulates that a *geoscientific site investigation programme* must be available before a site investigation begins. This programme is supposed to "specify the goals, measurement methods and evaluation methodology, as well as the acceptance criteria against which the site is evaluated". It is pointed out that site evaluation is a collective term for an interactive process consisting of different parts, as illustrated in Figure 1-1.

This report:

- identifies, describes and evaluates geoscientific "parameters" (see next section) which are of importance to know in order to be able to carry out *performance and safety assessments* of a deep repository based on the information that can be obtained from a site identification,
- presents and discusses the data needs for *planning and design of the rock works*,
- presents and discusses the data needs for description of *other environmental aspects*,
- presents other data needs for analysis and a general *understanding of geoscientific conditions.*

Figure 1-2 illustrates how this information – along with a planned description of measurement, interpretation and analysis methods – comprises an essential body of background material for the geoscientific site investigation programme.

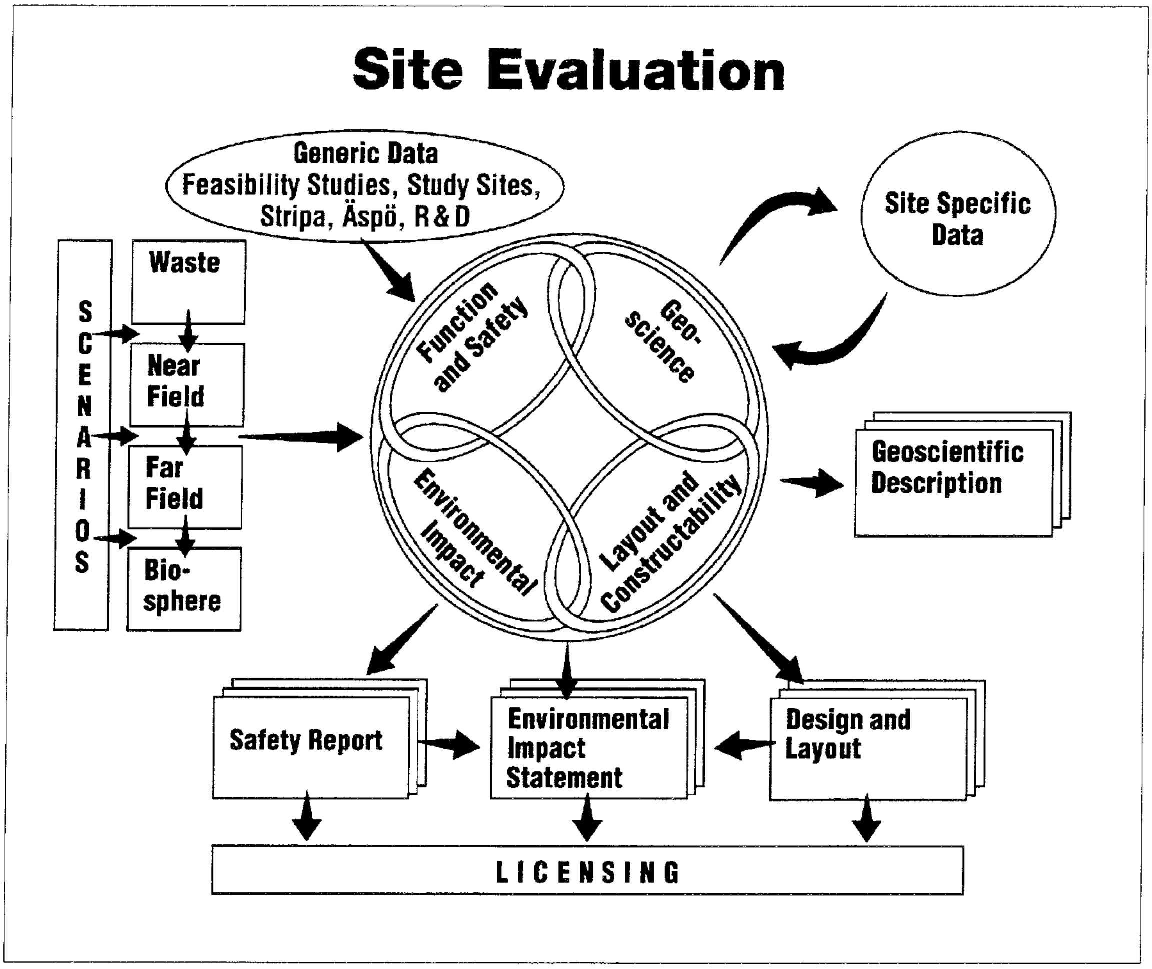


Figure 1-1. Scope of site evaluation (from SKB RD&D-95).

Another intention is that this document can be utilized to:

- define with greater precision the acceptance criteria against which a site is evaluated.

It is thereby verified that the parameters identified in this document include the so-called "siting factors" defined in the supplement to RD&D Programme 92 (SKB, 1994), even though certain parameters are reformulated, described in greater detail, or new.

The document further attempts to provide:

- a more detailed description of how different parameters influence safety performance, and how they are evaluated.

Finally, a supplementary goal is to clarify the information processing that takes place with data so that they can be utilized in the evaluation of a site's suitability. This clarification has been necessary to arrive at meaningful parameters, but should also be able to provide guidance in the planning of a future site evaluation.

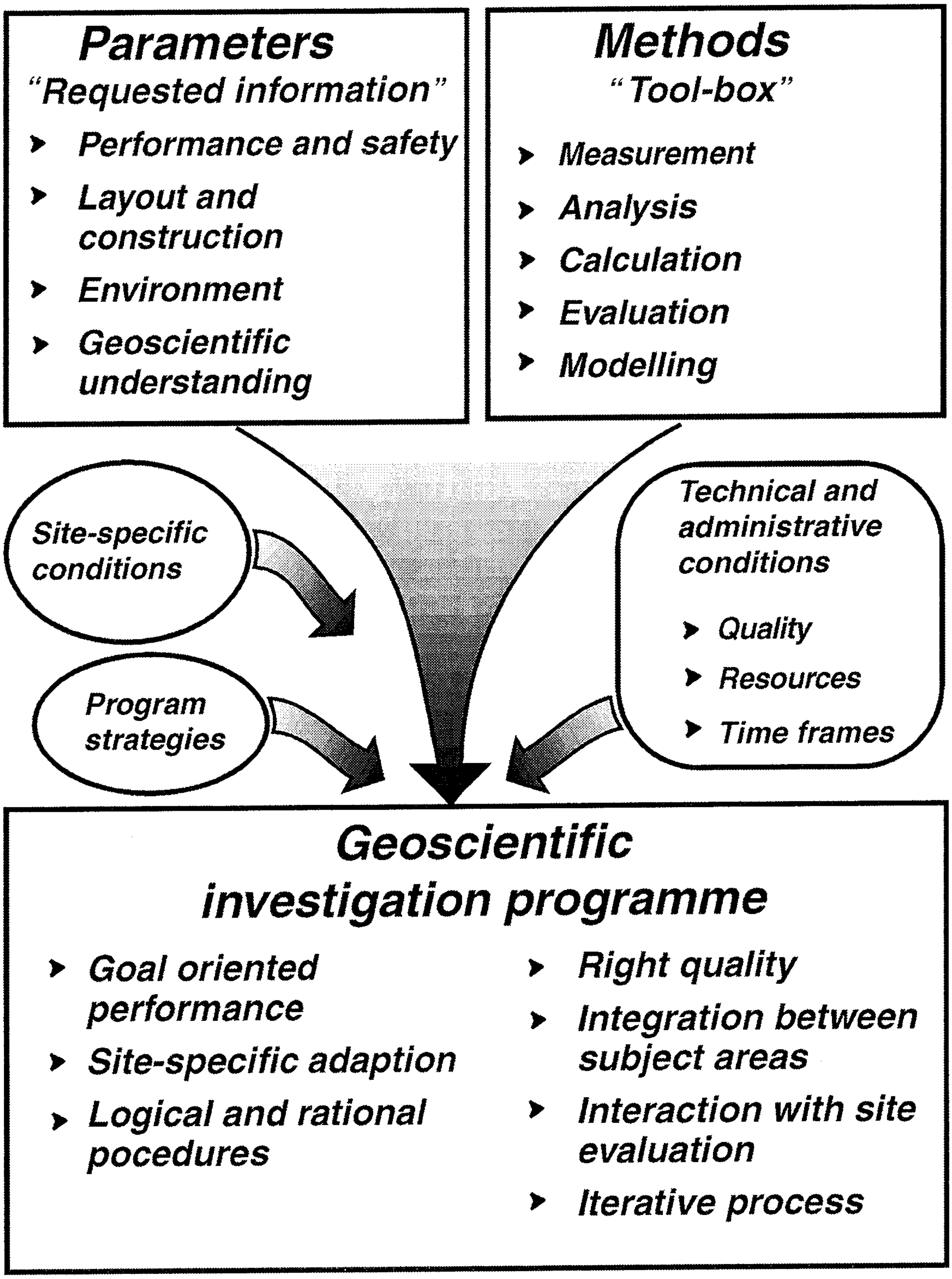


Figure 1-2. Schematic description of the background material that is needed for a geoscientific investigation programme. This report corresponds to the box headed "Parameters".

A planning of information processing is needed not least because it provides a basis for dividing the work into stages and for drawing up meaningful timetables for the geoscientific investigation programme.

1.1.2 The term "parameter"

The term "parameter" has been given a very broad interpretation in this work and cannot be directly translated to specific data for a given conceptual model. Within the Äspö project, Olsson et al. (1994) have developed a common structure for presenting and describing different models, where a model can be divided into *conceptual model*, *data* and *mathematical tools*. The conceptual model concerns the geometric configuration and the description of constituent processes, while data are used for quantification of the conceptual model. In other words, the conceptual model describes how the model is designed and contains no data.

In planning a site investigation programme, the difficulty arises that the site investigation can only partially aim at directly obtaining data for given conceptual models; another purpose is to identify conceptual models. In some cases, alternative conceptual models may also be applicable, in which case it should be possible to use the measurements to determine data for the different conceptual models. A planning document of this kind cannot one-sidedly describe input data needs for specific conceptual models in those cases where these uncertainties prevail. In cases where uncertainties can be assumed to prevail regarding which conceptual model should be used, the term "parameter" as used in this document is therefore given a more general meaning so that the physical/chemical conditions referred to can be described with various possible conceptual hypotheses. As a rule, the different data with which the parameter is described in different conceptual models is also discussed in this context.

1.1.3 Strategy

In order to be able to draw up and evaluate the parameter lists, the working group has – for the reasons put forth below – found it essential to distinguish between the *evaluation* of whether a site is suitable, the information that is needed to construct a *geoscientific model* of a site, and the data that can be obtained from practically available *measurement methods*.

- A *geoscientific model* of a site should be as objective a description as possible of what is known, including uncertainties, of the properties of the site on the basis of measurements performed. An important aspect of a site investigation and devising a geoscientific model is combining information from different measurement methods, as well as from different disciplines, in order to obtain a consistent picture of what the site looks like. In this work it is not possible to make use of simplifications and conservative assumptions; lacking information must instead be handled as uncertainties. With the geoscientific model as a point of departure, simplifications are subsequently made when evaluating the suitability of the site. The evaluation of a geoscientific parameter therefore often needs to take place in different steps. The parameter is manifestly essential if it directly influences parameters that are used in safety and performance assessment, but a parameter can also be essential if it is important in the construction of a geoscientific model. The primary emphasis in the present document is on *describing* and *evaluating* the *identified* geoscientific parameters.

- *The evaluation* of a site's suitability, and in particular models for performance and safety assessments, rarely uses directly measured data. As a rule, parameters obtained from a geoscientific model of the site are used. Furthermore, simplifications and conservative assumptions are used in the evaluation, since the purpose is to provide adequate safety margins as a basis for making a decision. One or a few critical parameters in the safety assessment may therefore be based on composite information from a large number of geoscientific parameters. Concepts used in adaptation of the configuration of the repository, for example "repository-discriminating discontinuities", comprise composite interpretations of the geoscientific model. The interpretations can further be based on results from the safety assessment. Methods and models for evaluation are discussed in the report under the heading *models and areas of application* for the various geoscientific disciplines.

- Few geoscientific parameters can be measured directly. This gives rise to various errors, one being measurement error, but above all upscaling problems and conceptual uncertainties. The relevance of different geoscientific parameters therefore needs to be considered in relation to the methods of measurement and evaluation that are available for determining the parameter. To shed light on this relationship, the document comments in certain cases on measurement methods in conjunction with the parameter description, even though the planning of the measurement programme will be dealt with in future documents.

In summary, it can be concluded that how the rock is to be described and which parameters are to be used depends on the purpose of the description. Furthermore, as a rule different individuals are responsible for designing the repository, carrying out safety assessment calculations and interpreting measurements from a site to a geoscientific model.

The working group has tried to focus on the information need that is expressed in published documents on safety assessment, primarily SR 95, although other information has also been utilized. The work has thereby to a large extent entailed documenting and compiling *already identified* parameter needs, information channels and information processings. A joint compilation of such information does not appear to have been done yet, however. In cases where an already documented evaluation is lacking, the evaluations offered in the document are based on assessments by the members of the working group, on viewpoints from various experts at SKB, and on viewpoints proffered at a workshop held in the autumn of 1996.

1.2 Performance and safety assessment

It is really not possible to stipulate all the parameters that are needed for a performance assessment and a safety assessment, since each investigated site (or studied layout) may have positive or negative features which need to be evaluated specially for this site (or layout). In the main, however, it is possible to specify, at least in general terms, which parameters actually influence containment performance and radionuclide transport in safety assessment calculations for a final repository of the KBS-3 type located at a depth of about 500 m in the Swedish crystalline bedrock.

1.2.1 Parameters in calculations in performance and safety assessments

During the work with SKB 91, lists were drawn up of what input data are used by the different models in the assessment. The lists, which are arranged parameter by parameter for the individual models, contain a general reference to process data, a description of how data is determined by classification as M (measured), E (expert judgement), K (generic knowledge) and I (interpreted), plus a qualitative assessment of parameter uncertainty and variability and their influence on barrier performance. The models and principles on which future safety assessments will be based are described in general terms in SR 95. Together with experience gained in other programmes, mainly SITE-94 (SKI, 1996) and TVO-92 (Vieno et al., 1992), this information has comprised a basis for judging which parameters need to be determined based on interpretation of a geoscientific model.

It should be observed that a safety assessment includes more than quantitative calculations of leakage, radionuclide transport and consequence calculations. Important site-specific properties may instead be of the type that determine whether the premises of the quantitative analysis are applicable. A supplementary way to describe the safety-relevant features of a site may, for example, be to evaluate the conditions for containment, retention, dilution and predictability.

In view of the fact that SKB's safety assessment work has developed, especially within the framework of SR 97, the information utilized by the working group regarding safety-relevant site-specific conditions should be augmented, for example in the manner proposed in the following.

- Set up tables for all quantitative models dealt with in SR 97 and describe how data for the models are obtained (and by whom).
- Evaluate the need for supporting site-specific data to justify (validate) the conceptual models used in the quantitative analysis.
- Analyze information needs that lie outside the so-called calculation chains, regarding both preconditions for analyses performed and information that may be needed to analyze different scenarios. Information on this could, for example, be obtained by evaluation of RES matrices.

The present document should therefore, if not before, be revised based on experience from SR 97.

1.2.2 Favourable, unfavourable and discriminating factors

The *favourable*, *unfavourable* and so-called *discriminating* factors discussed in the supplement to RD&D-Programme 92 (SKB, 1994) are presented in the document under the appropriate discipline. By discriminating factor is meant a condition that may occasion abandoning a site where site investigation has been commenced.

Since the RD&D supplement, no targeted activity has been carried out to further define or evaluate these factors. The review in this document shows, however, that these factors can be described with the parameters presented here. The parameter lists could therefore be used together with this document as a point of departure for a more specific discussion of site selection factors. The review also shows that previous judgements may need to be revised.

It can be observed that there are very few readily identifiable factors which by themselves could be discriminating. The suitability of a site is generally determined on the basis of a collective assessment of safety and constructability and can therefore not be determined until a complete site investigation has been carried out and evaluated. The term "discriminating factors" is nonetheless useful as a decision-making criterion for a site investigation, even though the absence of discriminating factors is not in itself any guarantee that the investigated site is suitable. At the same time, it should be made clear that the evaluation of a site's suitability cannot be limited to a search for discriminating factors. The term "site selection factors" should also include a description of which factors need to be measured on a site and how the measured information is to be evaluated. The present document should prove useful for this purpose as well.

1.3 Parameters for a geoscientific model description

The geoscientific analysis is divided into the following disciplines: *geology*, *rock mechanics*, *thermal properties*, *hydrogeology*, *groundwater chemistry* and *transport properties*. A number of parameters can be identified within each discipline to describe the properties of the rock.

1.3.1 Geoscientific parameters of importance for long-term performance, radiological safety and geoscientific understanding

Figure 1-3 illustrates the parts of the deep repository and their most important safety functions: *isolation*, *retardation* and *biosphere conditions*. The purpose of the geoscientific analysis is to provide data for parameters that can be used in quantitative consequence calculations regarding these safety functions, but also to build up a geoscientific understanding. The latter is important because a good understanding improves the credibility of the data that are used directly in

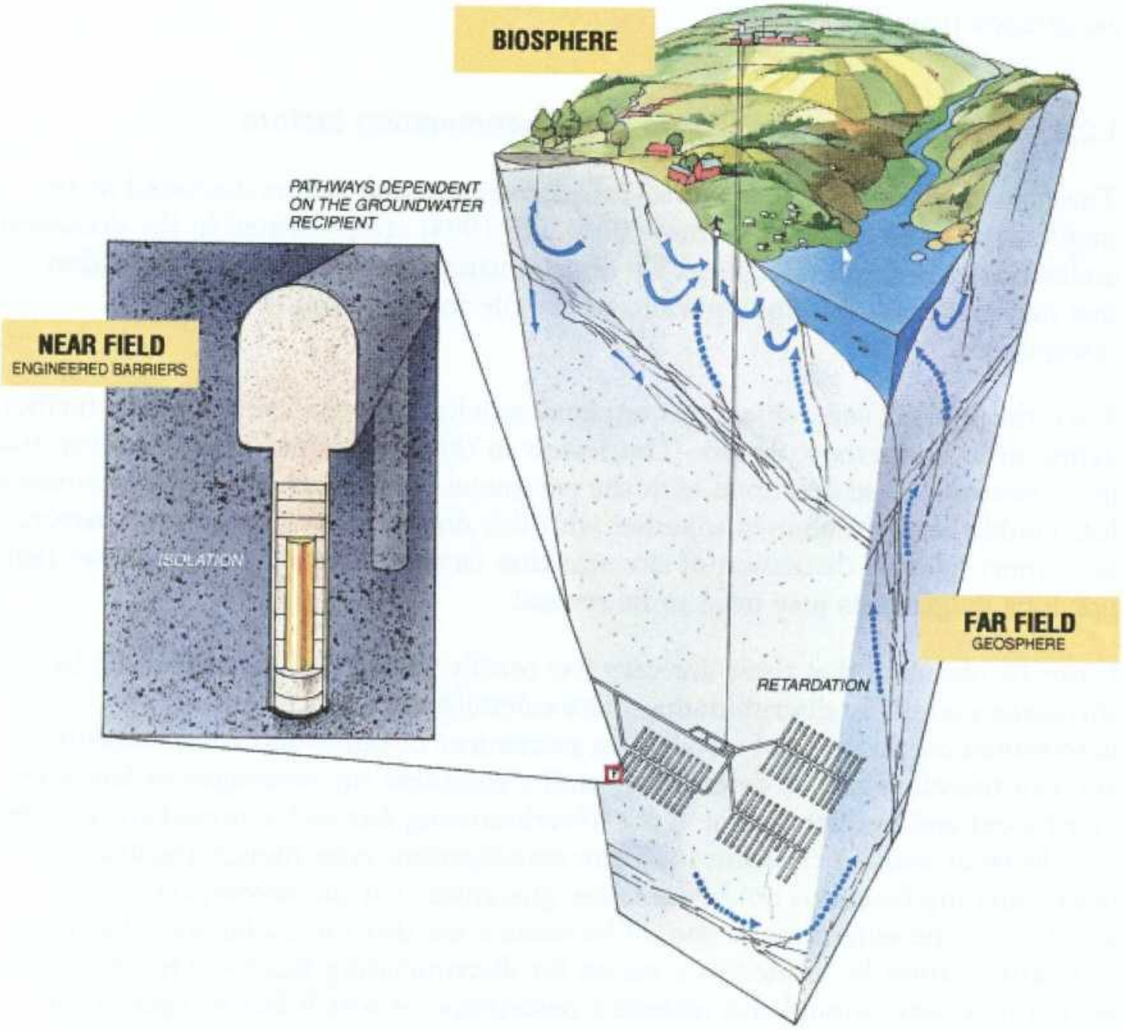


Figure 1-3. Parts of the deep repository and their most important safety functions (from SKB RD&D-95).

consequence calculations. Both of these purposes are essential for being able to carry out a site-specific safety assessment.

The descriptions of the rock given in different geoscientific disciplines should be consistent with each other. An attempt has therefore been made to establish which parameters should be described in the same way within the different disciplines and which can be identified freely within each discipline. This is above all important in the description of discontinuities in the rock.

The need for different parameters and the need for precision depends on which parameter values in the safety assessment need to be determined and justified. Data that are needed within a given geoscientific discipline may sometimes constitute an interpretation of information from another discipline.

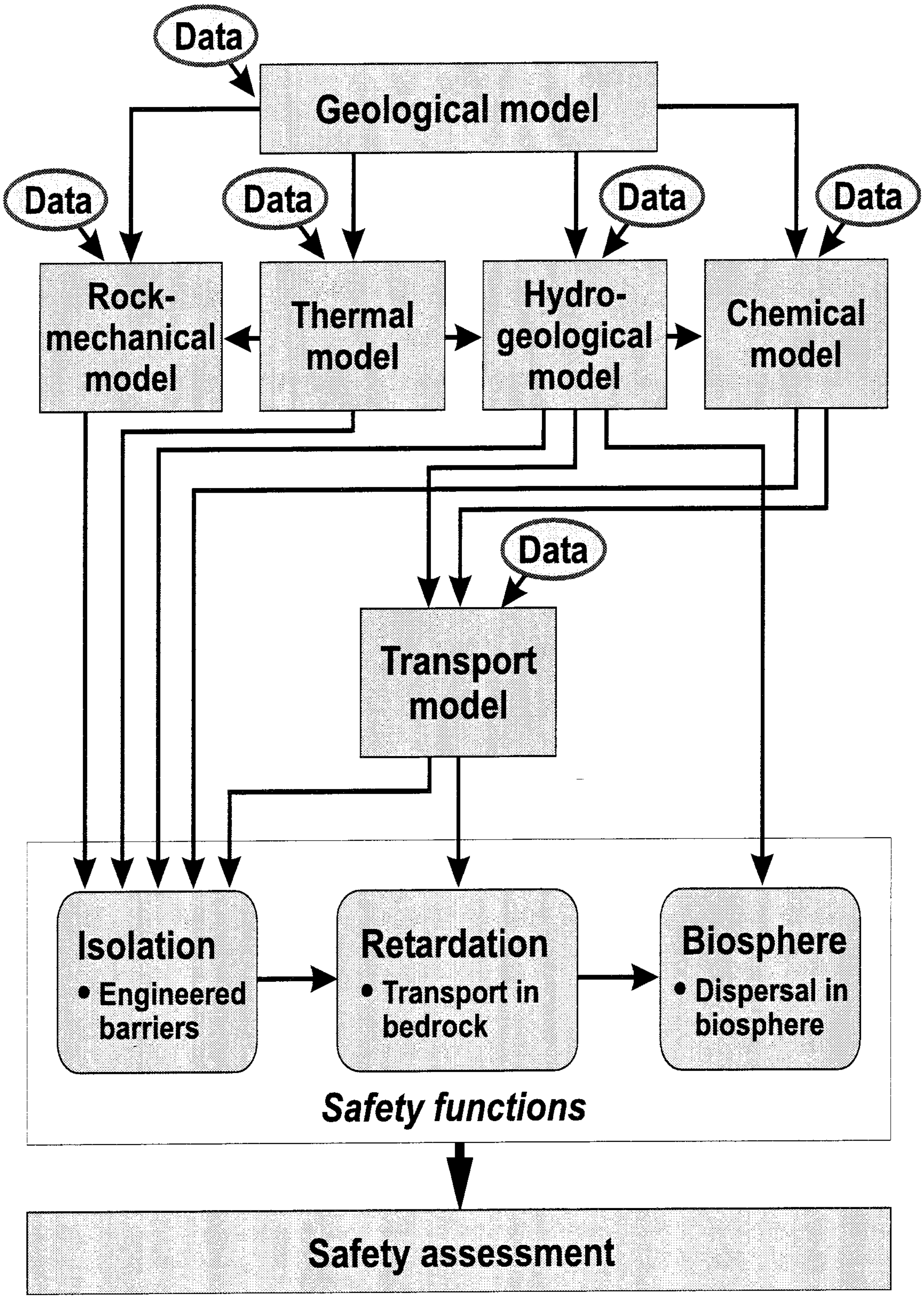


Figure 1-4. Schematic illustration of how information is transferred between different geoscientific models and how these models are utilized for safety and suitability assessment.

Hydrogeological and rock-mechanical models, for example, utilize structure-geological information, while the rock's retention properties are dependent on both hydrogeological and chemical conditions. This is illustrated in Figure 1-4. To enable data needs within each discipline to be derived, this leads to some repetition in the summarizing tables included in the document.

Wherever possible, geoscientific parameters should be described with the same nomenclature within different geoscientific disciplines. There is, however, no universal nomenclature regarding fractures and zones in the rock. Almén et al. (1996) have however proposed a nomenclature for such structures. This document uses the terms proposed there. This nomenclature is also explained in Chapter 2.

1.3.2 Data needs in planning and design of the rock works

The identification of geoscientific parameters has also been checked against the preliminary compilation of data needs that has been done for planning and design of the rock works (Windelhed and Alestam, 1996). If the same parameter is required for both construction analysis and safety assessment, it should be possible to coordinate measurement and to some extent also evaluation of this parameter.

The identified parameter requirement for planning and design of the rock works is presented under the relevant discipline in the document below. As a rule, however, information from Windelhed and Alestam on why different parameters are required is lacking – even though this is often relatively obvious. Furthermore, additional parameters that should be of importance for planning and design of the rock works have been identified during the work.

It can be concluded that the information needs of planning and design of the rock works are largely covered by the need for geoscientific information. It should therefore be possible to coordinate information gathering during the site investigation so that both design needs and geoscientific needs are met. This requires good planning, of course. This document, along with Windelhed and Alestam (1996), should be able to be used for such planning.

Finally, it should also be noted that a construction analysis is based on practical experience of utilization of site-specific data, and that SKB will be the principal judge of whether the construction analysis is sufficiently comprehensive, even though it must of course be possible to demonstrate that operation (and progressive construction) of the deep repository can be carried out in a safe manner. Other demands will be made on the data that are used to furnish parameters for performance and safety assessment, experience feedback is lacking, and these demands will be made not only by SKB but also by the regulatory authorities.

1.3.3 Other environmental aspects

The document also discusses in general terms data needs for description of land and environment (other environmental aspects). The need for information here is driven above all by future demands on assessment of the repository's environmental impact aside from ionizing radiation. The impact on the (near-surface) environment from a radiation protection point of view will also have to be assessed (SSI, 1995). Relevant information in this respect is already being collected in ongoing feasibility studies, and there may therefore be occasion to revise this document on the basis of experience from feasibility studies and ongoing EIA consultation.

1.3.4 Evaluation of parameters

The emphasis in the work has been on identifying parameters and describing how they are used. An evaluation of the importance of the different parameters is also made in the document. This evaluation is also presented in abbreviated form in the tables in Appendix A. The evaluation is divided into a number of main headings and sub-headings to illustrate the importance of the parameters with respect to:

- *Long-term performance* and *radiological safety*; divided into isolation, retardation and biosphere. Isolation is in turn divided into canister, bentonite, rock and intrusion. Retardation is divided into fuel, canister, bentonite, groundwater flow in rock and retention in rock (see also Figure 1-3).
- *Design*; divided into layout, construction analysis and working environment.
- *Other environmental aspects.*
- *Geoscientific understanding.*

It is also indicated whether the importance is essential (E) or limited (L). Importance is given for those functions that are most immediately affected by the parameter (directly or indirectly). The evaluation is based on expert judgements carried out in the manner described in section 1.1 above. It should be emphasized that the evaluation (E or L) is subjective and that the working group has concentrated the work on identifying and describing parameters rather than evaluating them.

By "isolation" is meant the barrier's ability to contain radionuclides. Strictly speaking, such an ability is only possessed by the canister (and the rock against intrusion). The columns "bentonite" and "rock" pertain to whether the parameter can contribute to a change in the properties of the barrier. By "retardation" is meant the barrier's ability to retard the transport of any released radionuclides. For example, Table A:4 indicates that the permeability distribution of the rock has an essential influence on the size of the groundwater flow (ought to be obvious), and an essential influence on retention in the rock (which is directly dependent on the flow). It is further indicated that the permeability distribution has a limited influence on the isolation of the canister (influx of corrodants) and can also have a limited influence on the stability of the bentonite (through erosion if the flow is substantial) (see further Chap. 5).

It should be emphasized that the evaluation shown in the tables is intended to provide an overview of the information that is discussed in this document. It is not possible to describe all essential aspects of a parameter in tabular form. For example, the table cannot show that a parameter may be very important to know with great precision in one part of the repository area, but not in others. Nor is the division between the isolating function of the rock and its retarding function clear-cut. The distinction between essential and limited is not an obvious one either and varies between geoscientific disciplines and the different cases that may have to be analyzed in the safety assessment.

1.4 Measurement methods

How desired parameters can be measured is discussed in general terms in the document. This is to be regarded as an introduction to the work that needs to be done to identify which measurement methods are to be used and how they are to be evaluated.

1.4.1 Coupling between measurement methods and possible parameters and generic data

The reason measurement questions are dealt with in this document is the strong coupling between geoscientific modelling and practically feasible measurement methods. It would be meaningless to draw up a list with completely unrealistic demands on data (for example a total determination of the inherent properties of all fractures). A reasonable list of demands on geoscientific information needs to be based on a compromise between what is desirable and what is feasible. An important limitation is that many geoscientific parameters cannot be measured directly. Most tests that are performed in the field (e.g. injection tests, hydraulic fracturing, tracer tests etc.) provide indirect information on e.g. hydraulic conductivity, rock stresses or retention properties. Evaluation, interpretation and analysis of site-specific measurements therefore comprise a part of the geoscientific analysis.

Another question to discuss in this context is whether it is at all meaningful to determine certain parameters site-specifically either because they are well known (for example thermal properties of the water) or because the uncertainties are so great that it cannot be expected that today's measurement methods applied on a given site will yield results which significantly differ from results from other sites (which can be the case for the "flow-wetted surface").

Such data is often somewhat erroneously called "generic" or "non-site-specific". It should be made clear that the use of "generic" data is not a problem as long as they offer the best site-specific prediction of the parameter. That different sites have the same "generic" data is merely an expression of the fact that different sites do not differ with regard to this parameter (which, for example, is obviously true for the properties of the water). There is, on the other hand, reason to question the quality of generic data; are they based on a defensible procedure, or merely a repetition of values used in previous modelling? If generic data are used, the following questions therefore need to be raised and answered:

- Are the values used representative of the site, and are measurements needed to confirm this?
- Is the uncertainty associated with the data too great for them to be used in the safety assessment?
- Is there potential for improvement, either by use of a better "generic" value or by introduction of more site-specific knowledge?

These questions should be analyzed in later stages in the development of a site investigation programme. This report merely notes when the use of generic data may be considered.

1.4.2 Choice of measurement method – geoscientific investigation programme

In view of the strong coupling that exists between choice of measurement methods and possible geoscientific parameters, it is important to check that the parameters asked for in this document are matched by actual methods for measurement and evaluation. Compilations of measurement methods have already been published (see e.g. Almén et al., 1994) and they are also collected in a preliminary measurement method table. A conceptual sketch of the scope of an initial site investigation is also presented in RD&D-Programme 95 (SKB, 1995) (Figure 1-5).

However, previously done compilations should be combined with this document and other experience, for example from comparisons between pre-investigations and investigations from the construction phase of the Äspö Hard Rock Laboratory (see for example Rhén (ed.), 1996). For each parameter/discipline in the parameter table, it is therefore necessary to shed light on:

- which measurement method is to be used,
- how "many" measurements need to be done (e.g. number of boreholes, resolution along the borehole, etc.),
- how the measurement method should be evaluated and with what degree of (un)certainty the substance/parameter can actually be determined with the aid of a given method,
- whether the proposed measurement method(s) are influenced by other measurements.

Such a document would represent an important step towards the realization of a geoscientific investigation programme.

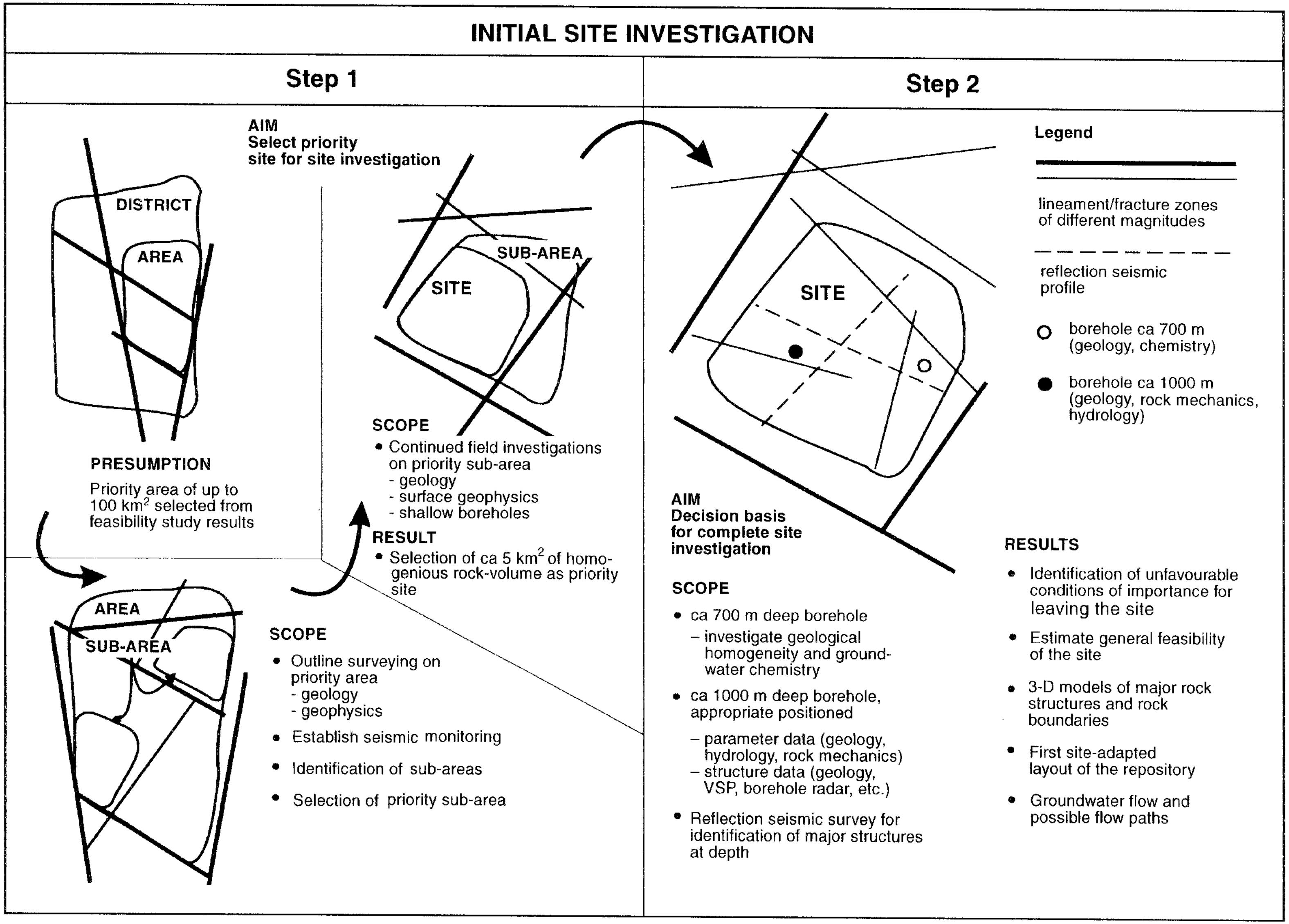
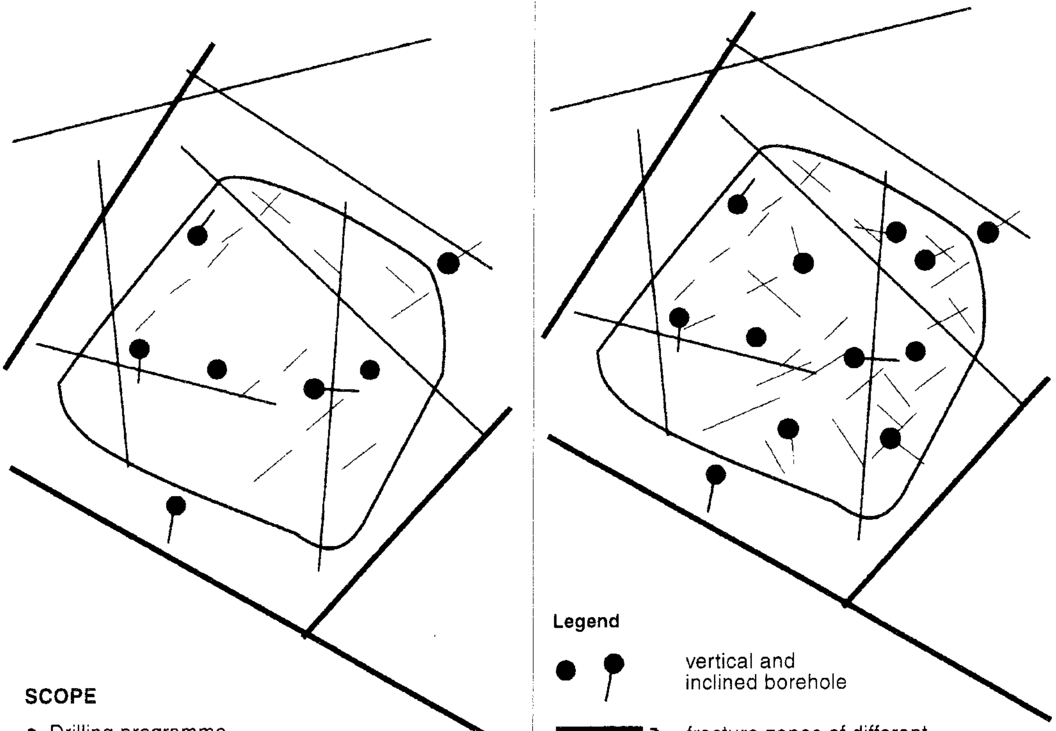


Figure 1-5, a. Conceptual sketch of scope of initial site investigation presented in RD&D-Programme 95. This sketch may have to be revised on the basis of the information presented in this report.

COMPLETE SITE INVESTIGATION

Step 1 | **Step 2**

AIM
Basis for application for detailed investigations



Step 1

SCOPE

- Drilling programme
  - extension and properties of rock types, including dykes
  - position and properties of fracture zones of major importance
  - frequence and properties of fracture zones of less importance

RESULTS

- Basis for performance assessment and design
  - preliminary layout (D2) adapted to site conditions
  - decision of repository depth, tunnel/shaft
  - construction analysis
- Basis for groundwater modelling
  - groundwater flow velocities
  - identification of discharge areas

Step 2

SCOPE

- Drilling programme
  - extended knowledge and increased detailness of parameter data on rock types and structures (extension, properties etc.)
  - in-situ measurement of groundwater flow
- Regional environment
  - supplementary investigations for verification/adjustment of groundwater flow model
- Special issues
  - Complementary investigations and studies

RESULTS

- Basis for performance and safety assessment and design
  - analyses of longterm radiologic safety for different modelling alternatives and parameter sets
  - adjusted site-adapted layout of the repository

Figure 1-5, b. Conceptual sketch of scope of complete site investigation presented in RD&D-Programme 95. This sketch may have to be revised on the basis of the information presented in this report.

2 Geology

2.1 Overview of parameters, methods and areas of application

Table 2-1 summarizes which data are primarily needed to be able to construct a geological model. The table also attempts to show examples of which measurements can be used to estimate the parameters and how they are used. The parameters in Table 2-1 are also included in the collective parameter table in Appendix A:1. (Examples of general references to what can constitute suitable geological parameters are Gustafson et al., 1991 and Bruun et al., 1992).

Table 2-1. Overview of data requirements for geological description, examples of measurement methods and areas of application.

Parameter	Method	Used for
Topography	Maps, terrain elevation data	Overview, structure-geological model, identification of structures.
Soil layers ***Soil types*** – thickness of soil cover – soil type distribution – soil type description – soil – bottom sediment – indication of neotectonics	Mapping, drilling/probing, geophysics, sampling, lab studies	Soil type model (Indirect land and environment, superficial hydrogeology, biosphere model) assessment of neotectonics.
Lithology ***Lithological structure*** – rock type distribution (spatial and percentage) – xenoliths – dikes – contacts – age – ore potential – industrial minerals	Mapping, geophysics, drilling, lab studies	Lithological model (used indirectly for rock-mechanical, hydrogeological and geochemical understanding).
Rock type description – mineralogical composition – grain size – mineral orientation – microfractures – density – porosity – susceptibility, gamma radiation etc. – mineralogical alteration/ weathering	Sampling, lab studies, field studies geophysics, borehole logging	Lithological model (used indirectly for rock-mechanical hydrogeological and geochemical understanding).

cont'd. on next page

Parameter	Method	Used for
Structural geology ***Plastic structures*** – folding – foliation – lineation – shear zone – veining – age	Geological mapping, laboratory analyses of drill cores, etc.	Structure – geological model.
Brittle structures – faults – fractures (fracture zone) – age	Geophysics, geological mapping, drilling, analyses of drill cores, etc.	Structure – geological model.
Properties of discontinuities (Brittle and plastic structures of mechanical importance) Regional and local discontinuities – position – orientation – length – width – movements (size, direction) – genetic type – inner properties (number of fracture sets, spacing, block size, fracture roughness, fracture filling (fracture mineral), alteration, weathering	Geophysics, geological mapping, drilling, lab test, interference test	Structure-geological model. Repository design. Input data to hydrogeological model and rock-mechanical model. Fracture minerals and other input data to geochemical model.
Local minor discontinuities (mainly data that permits stochastic description of parameters, but where discrete observations are reported) – position (spacing) – orientation – length – width – movements (size, direction) – inner properties (number of fracture sets, spacing, block size, fracture roughness, fracture filling (fracture mineral), alteration, weathering	Geophysics, geological mapping, drilling, lab test, interference test	Input data to hydrogeological model and rock-mechanical model (repository design). Fracture minerals and other input data to geochemical model.
Fractures – data that permit stochastic description of – spacing (different sets) – orientation – persistence (length) – contact pattern – aperture width – roughness – filling (fracture mineral) – alteration, weathering (wall strength	Mapping of outcrops, drill cores (tunnels in latter phases)	Input data to detailed hydrogeological model and detailed rock-mechanical model. Indirect input data to nuclide transport model. Fracture minerals and other input data to geochemical model.

2.2 Models and areas of application

The geological information is used to formulate a *geological model.* The geological model is descriptive and is formulated to compile geological information in a structured and consistent manner. A special format has been adopted within the Äspö project for how the geological model is to be described (Olsson et al., 1994, p. 14). This format appears to be directly applicable to the set of parameters given in Table 2-1.

The purpose of a geological model is to describe the soil cover and the properties of the bedrock within a given area as realistically as possible. As a rule, the geological model is not used directly for safety assessment, but primarily used to provide input data to the rock-mechanical, hydrogeological and geochemical models (see e.g. SR 95, pp. 70–77 of the English version). Furthermore, the geological model serves as a basis for the geoscientific understanding of a site.

From a practical point of view, it may be useful to divide the geological model into a *soil type model,* a *lithological model* and a *geological structure model.* It should be pointed out that these models are interrelated, comprising parts of one and the same geological model, and that efforts should be made to keep the different parts of the geological model consistent. A *geological evolution model* is also needed as a basis for understanding these models and how they are related. The structure and use of the geological model is illustrated schematically in Figure 2-1.

2.2.1 Geological evolution model

The geological evolution model comprises the basis for the geoscientific understanding of the geology of the site. The evolution model describes how the area was formed and evolved historically. The age data reported among the various parameters, obtained for example from isotope measurements, comprise an important source of information here.

2.2.2 Soil type model

The soil type model describes above all the distribution, thickness and composition of different soil types and sediments. This model primarily serves as a basis for the modelling of near-surface environmental consequences and receptor conditions (biosphere modelling), which is discussed in greater detail in Chapter 5. However, indications of e.g. neotectonic movements influence the assessment of the suitability of a site from a long-term mechanical viewpoint.

2.2.3 Lithological model

The lithological model provides a description of the lithological structure of the rock mass as regards the distribution of different rock types in both spatial and percentage terms, plus a characterization of the different rock types. This model is

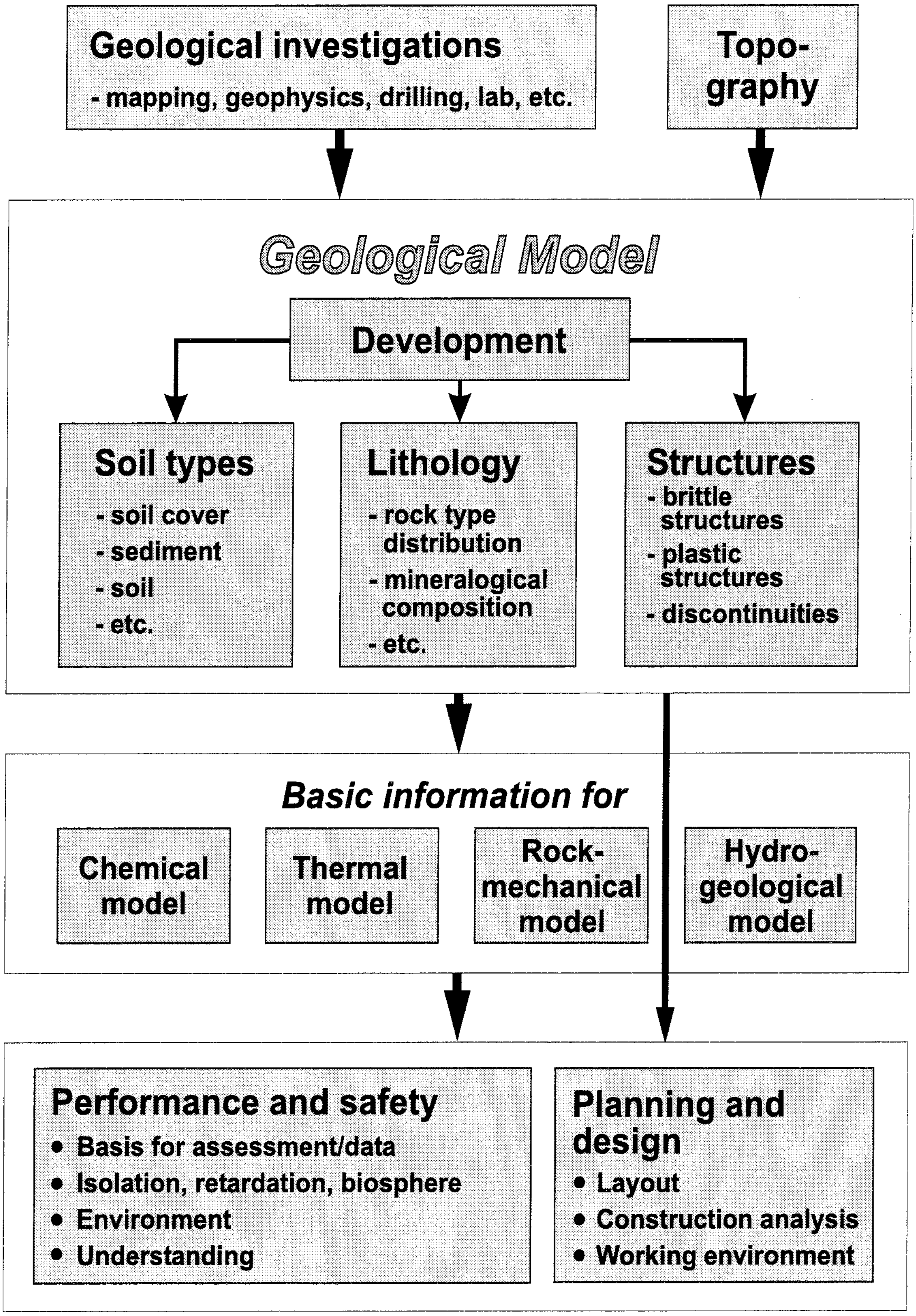


Figure 2-1. Schematic illustration of structure and use of the geological model.

primarily of importance for interpretation of the structure-geological and rock-mechanical models. Lithology is also of importance for a geochemical understanding of the site (see Chapter 6). According to the supplement to RD&D-Programme 92 (SKB, 1994), the occurrence of ore is identified as an unsuitable condition and can also be discriminating in the sense that it leads to abandonment of the site. Figure 2-2 shows an example of a preliminary lithological model of the Äspö area. For certain applications, however, the resolution in the model needs to be much greater than that indicated by the figure.

2.2.4 Geological structure model

The geological structure model describes both the plastic structures in the rock mass, e.g. folding and foliation, and the brittle structures, e.g. fractures and fracture zones, which are summarized under the designation "discontinuities". The geological structure model is of direct importance for rock-mechanical and hydrogeological models, as well as for engineering-geological predictions and general geological and hydrogeological understanding. The geological-structure model is also of very great importance for the design of the deep repository, since the principles that are used today for placement of the deep repository are based to a high degree on fitting-in according to the principal discontinuities.

2.2.5 Favourable, unfavourable and discriminating factors

In the supplement to RD&D-Programme 92, a number of geological factors were rated as favourable, unfavourable or discriminating.

The following factors were rated as *favourable*: A common rock type without interest for other utilization of natural resources, a large site with few major fracture zones, homogeneous easy-to-interpret bedrock, and few fracture zones with a low to moderate fracture frequency. *Unfavourable* factors were said to be: highly heterogeneous and difficult-to-interpret bedrock, known deformation zones and postglacial faults, rock types that might be of interest for prospecting. Factors rated as *discriminating* in the sense that they can occasion abandonment of a site where site investigation has begun were: valuable ores or minerals in the repository area and many closely-spaced water-bearing fracture zones. These factors obviously need to be more precisely defined to be directly useful as discriminating factors.

The geological parameters identified in the following sections include all the parameters noted above. Some terms are given a stricter definition here, however (e.g. "structures" are termed "discontinuities", see below). The above evaluation probably needs to be revised. A more exact definition and possible revaluation of site selection factors based on the geological model can be based on the parameter list in Appendix A:1.

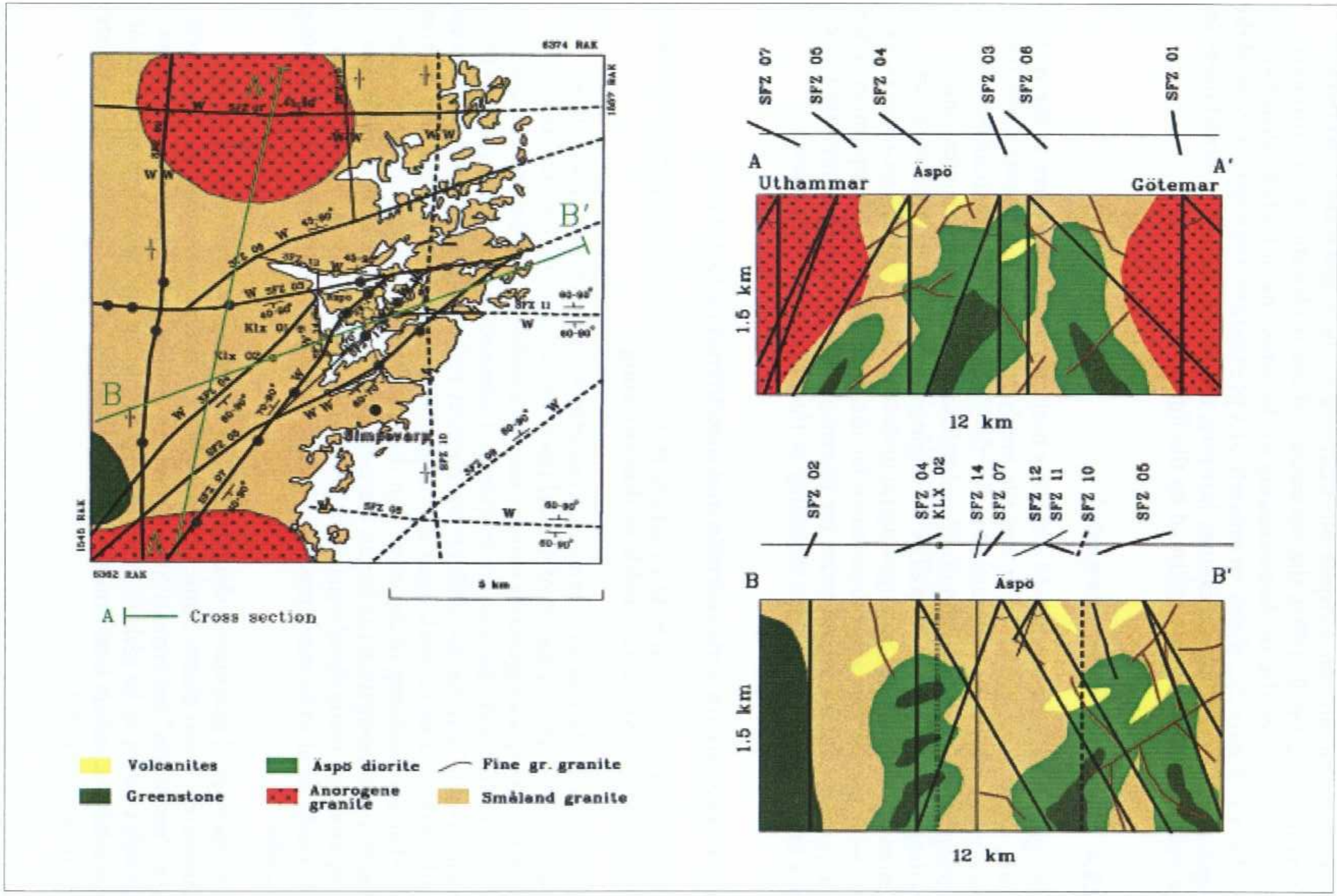


Figure 2-2. Example of lithological model on regional scale (from SKB SR 95).

2.3 Topography

Topography, including other surveying-related information such as cartography and geodesy, provide essential information on a site.

The topography of the investigated area is of obvious importance for being able to build up a geological model of the site. It provides an overview, it is utilized for identification of structures (see Almén, 1994) and it is utilized to formulate hydraulic boundary conditions (see Chap. 5). The evaluation below can also be found in the table in Appendix A:1.

Detailed topographical information is utilized to identify discontinuities on different scales. The information is therefore indirectly of essential importance for the rock's isolating properties and for the groundwater flow in the rock. High resolution is required.

On a regional scale, topography also affects, via boundary conditions, the groundwater flow in the repository area. Seabed topography is also of importance in this respect for being able to judge the impact of sea level changes. On a smaller scale, however, the local topography in the repository area is of minor importance for the groundwater flow at repository level (see Chap. 5).

Relevant topographical information has probably been collected in conjunction with feasibility studies and should thereby be available in the height database. However, this information needs to be supplemented in conjunction with a site investigation in order to provide a higher level of detail.

2.4 Soil types – distribution

Information on soil types is used to devise a soil type model. This model is used above all to model near-surface environmental impact and receptor conditions. Appendix A:1 also shows how the different parameters are evaluated in terms of importance.

The thickness of the soil cover and the grain size of the soil types (which can be derived from the soil type distribution and the soil type description) furnish indirect information on the size and properties of the water-bearing strata. In cases where greater precision is needed in the near-surface groundwater modelling, the soil type information needs to be supplemented with hydraulic information. For modelling of receptor conditions (biosphere modelling) and for other description of the near-surface environment, this information is of limited and indirect importance. The occurrence/thickness of bottom sediments may be of essential importance in models for circulation of radionuclides released into the environment (biosphere models, see Chap. 7). Thickness and bottom sediments influence the boundary conditions for groundwater flow in the rock, but the influence is of limited and indirect importance. The information is of direct and essential importance for the geoscientific understanding of the site.

Thickness and soil type distribution are also of importance for repository layout.

The soil information is of limited importance for description of receptor conditions and the near-surface environment (see further Chap. 5).

Studies of the soil cover may reveal indications of postglacial movements (neotectonics). Since such movement should preferably not occur in a repository area, such observations are of essential importance for being able to assess long-term mechanical stability (isolating capacity of rock in Appendix A:1).

Measurement methods etc.

A general overview of the soil type distribution within an area can usually be obtained from existing map material. The soil layers (and bottom sediments) can also be investigated geophysically by seismic methods. Well data can provide supplementary information on soil depth. Information on soil type distribution and bottom sediments can be supplemented by drilling. Supplementary field mapping and drilling (digging of test pits) are needed for a more detailed soil type model. The soil type description is done largely based on data from laboratory investigations of soil samples.

2.5 Lithology and rock type description

Information on lithological structure and description of rock types within this structure are needed to formulate a lithological model. The evaluation below can also be found in Appendix A:1.

Lithological structure

The lithological model requires a description of the rock mass on a regional scale, mainly with regard to dominant rock types but also possible occurrence of dikes and xenoliths for determination of lithological homogeneity.

The properties of the rock types (rock type description) are of (limited) importance for mechanical stability as well as for geochemical properties.

The rock type distribution is of essential importance for layout and construction analysis (influences mechanical properties), but limited importance for the isolating function of the rock (mechanical properties) as well as for its retarding properties (retention).

Dikes and contacts affect rock strength and are therefore of essential importance for repository layout and construction analysis, but are of more limited importance for the isolating capacity of the rock. Dykes are also of essential importance for a geoscientific understanding of the site, while the contacts are in themselves of more limited importance. Estimates of age are of interest for geoscientific understanding (the evolution model).

Ores and industrial minerals in exploitable quantities are unfavourable factors for the site and are thereby of essential importance for assessment of intrusion, layout and geoscientific understanding. Their possible occurrence should therefore be determined early.

Rock type description

The mineralogical composition of the rock types, as well as mineralogical alteration/weathering, influence both the mechanical stability of the rock and the chemical environment. These parameters are therefore of essential importance for layout, construction analysis and working environment, and indirectly of limited importance for assessing long-term stability (isolation rock) and retardation.

For the chemical (geoscientific) understanding, which underlies the credibility of the chemical model (see Chapter 6), it is necessary to have a grasp of what minerals are contained in rocks and fracture filling, as well as indications of mineralogical alteration/weathering. This is especially true of relatively soluble minerals (e.g. anhydrite), minerals that are reactive in other ways (e.g. clay minerals), and those that could reveal the geological history of the area (e.g. iron (III) minerals). Indirectly, this information is also of limited importance for the retention properties of the rock.

The occurrence of microfractures and resultant porosity accessible for matrix diffusion is theoretically of great importance for the retention properties of the rock (see Chap. 7) but is, in view of uncertainties etc., in practice only of indirect and limited importance for this aspect. Microfractures scarcely influence hydrogeology.

The rock type description provides indirect information on the strength of the rock, although there are no absolute correlations (see Chap. 3). The grain size of the rock types is often of great importance. Fine-grained rocks such as fine-grained granites/aplites are normally brittle and highly fractured. Extremely coarse-grained rocks such as pegmatite and certain coarse-grained granites are often also rock-mechanically non-homogeneous. Mineralogical alteration/weathering is also a parameter of importance from a strength viewpoint. These parameters are thereby of direct and essential importance for layout and construction analysis, but of more limited importance for the isolating capacity of the rock.

Mineral orientation, along with various geophysical parameters such as susceptibility and gamma radiation, are primarily of importance for geoscientific understanding.

Measurement methods and need for resolution

Investigation of the rock's lithological structure mainly involves geological mapping and geophysics. It is supplemented by a number of cored holes to the relevant depth, which are positioned with the guidance of surface investigations. The parameters for the rock type description are determined by analysis of drill cores and various geophysical logs in the boreholes.

Although certain lithological parameters are of essential importance, the need for resolution is usually limited. As a rule, the information is needed on a relatively large scale. This means that the information needed for the lithological model should generally not determine where boreholes are positioned. However, as for other parameters (see following sections), it is essential that information be available on conditions where the repository will be located so that boreholes are not positioned solely to identify structures.

2.6 Structural geology

Over the course of millions of years the bedrock has been subjected to forces and temperatures that have partially melted and deformed it. At great depths in the earth's crust, where temperatures and pressures have been sufficiently high, this deformation has been plastic, i.e. without brittle fractures. In the upper, firmer part of the rock the deformation has been brittle (of a ruptural character), forming fractures and fracture zones. The geological structure model describes the structural make-up of the rock and is therefore based on information regarding both plastic and brittle structures. However, a strict classification of the structures into these categories is not possible, since transitional forms exist.

The geological structures are investigated in conjunction with geological field mapping. The necessary resolution is determined by site-specific conditions.

The term "discontinuity" is used above all for designating the brittle (ruptural) structures, but certain plastic structures are also included in the discontinuity concept, see section 2.7. Evaluation of the importance of the geological structures for the performance of the deep repository is shown in Appendix A:1, where the composite properties are above all taken up under the relevant discontinuity.

2.6.1 Plastic structures

A large part of the older bedrock in Sweden was deformed plastically between 1.5 and 2 billion years ago, when the superficial bedrock was situated at a depth of about 10–15 km with temperatures of about 250–350°C. As a result of this deformation, the bedrock was folded and different structures – e.g. folds, foliation, lineation and veining – were formed. One type of rock that was formed by alteration of other rock types in conjunction with this deformation is gneiss. Banded, very heavy deformation has resulted in persistent plastic shear zones. Mylonite is a rock type that was formed under banded strong deformation, mainly in conjunction with faults.

The plastic structures are chiefly of importance for interpretation of the deformation history of the rock mass and a general understanding of its structural composition. The disposition of brittle structures is largely controlled by previously formed plastic structures. Plastic structures of importance are above all shear zones, which are often associated with mechanically reduced strength and are therefore included in the discontinuity concept of importance for the layout of the deep repository, see section 2.7. Foliation, folds, lineation and veining often entail anisotropy (direction-dependent variations) in thermal and mechanical properties. This variation must be taken into consideration in calculations of e.g. induced rock movements in the repository. These structures also often control the small-scale fracture pattern and thereby indirectly influence permeability and connectivity between fractures. Dating is of importance for the geoscientific understanding of the site.

2.6.2 Brittle structures

The brittle (ruptural) structures have developed in a brittle rock mass and mainly consist of fractures or fracture zones that have formed in conjunction with faults and overthrusts, i.e. are mechanically induced, while other fractures are thermally induced.

Individual fractures and fracture zones occur with varying lengths and properties, often with a complex geometric structure. The fracture zones have often been formed in connection with primary plastic structures. They are normally characterized by heavy foliation, high fracture frequency with locally crushed or clay-altered sections and a varying degree of hydraulic conductivity. The properties of the fractures are largely controlled by the fracture surface's character, shape, possible mineral coating or other fracture filling and mechanical restraint.

The brittle structures are usually of great direct importance for the hydrogeological and rock-mechanical properties of the bedrock (see chapters 3 and 5) and thereby have a great influence on the isolating and retarding properties of the bedrock and on the layout of the deep repository.

According to SKB's classification system, all brittle structures are included in the discontinuity concept, see further section 2.7. The importance of the properties of the brittle structures for a deep repository is discussed further in this section.

2.7 Discontinuities

2.7.1 Nomenclature

In order to ensure uniformity of terminology, this document uses the nomenclature proposed by Almén et al. (1996). The term "discontinuity" is used as a generic term for all ruptural structures, i.e. fractures and fracture groups (fracture zones), and for certain plastic structures such as shear zones. By "discontinuity" is meant *any mechanically deviant structure, e.g. fracture, plane or zone of schistosity – usually extending in two principal dimensions – with a lower strength than its surroundings*. When defined in this manner, discontinuities can include everything from microfractures to regional zones of weakness. It should also be noted that with this definition the mechanically or mineralogically altered "wall rock" is also included in the discontinuity.

In connection with geoscientific characterization, the discontinuities are divided solely according to geometric size into regional discontinuities, local discontinuities, local minor discontinuities and individual fractures, according to Table 2-2. The table also shows the proposed level of ambition for description in the site investigations. Due to the complex structure and geometry of the discontinuities, the borderlines between the groups can be slightly fluid. For this reason, other geoscientific parameters can be taken into account when a given discontinuity is classified geoscientifically.

Table 2-2. Classification and naming of discontinuities and level of ambition in description in site investigation (after Almén et al., 1996) – the dimensions are approximate.

Name	Length	Width	Ambition in description
Regional discontinuities	>10 km	>100 m	Deterministic.
Local discontinuities	1–10 km	5–100 m	Deterministic.
Local minor discontinuities	10 m–1 km	0.1–5 m	Stochastic (some determin.).
Individual fractures	<10 m	<<0.1 m	Stochastic.

It should be emphasized that the lengths and widths shown in Table 2-2 are approximate. It should further be observed that the classification shown in Table 2-2 does not entail an evaluation of the properties or importance of the discontinuities. The purpose is to establish a nomenclature that can be used consistently in all geoscientific models. Within other geoscientific disciplines it is then possible to identify parameters that describe the properties of the discontinuities. Whether a given discontinuity is essential or not in some respect is thereby determined within each discipline.

For layout and analysis of the long-range safety of the deep repository on a site, it has also been proposed that the discontinuities can, after complete geoscientific characterization (i.e. after hydrogeological, rock-mechanical and chemical analysis), be divided into different functional classes D1–D4 (see Almén et al., 1996). In connection with functional classification, a major discontinuity can theoretically be assigned to a less important functional class, for example if it is not hydraulically significant, and a minor discontinuity can be assigned to a more important functional class.

2.7.2 Regional and local discontinuities

In view of the fact that the major discontinuities can be important for the mechanical and hydrogeological properties of the site, the site investigations should aim to locate all regional and local discontinuities deterministically. The risk that there might be undiscovered discontinuities of these sizes should also be estimated.

Large discontinuities can affect the placement or layout of the entire repository in accordance with the proposed functional classification, depending on what properties they have. This means that the geometric description – i.e. position, orientation, length and width – is directly of essential importance for the layout and construction analysis of the repository. Indirectly, these quantities are of essential importance for being able to judge the isolating capacity of the rock and for being able to judge the groundwater flow on a site scale (see Chap. 5). It is important to determine the extent of these discontinuities beyond the repository area as well. In the analysis of long-term pumping and tracer tests (LPT2) on Äspö Island, Gustafson and Ström (1995) conclude that the absence of such information gives rise to interpretation uncertainties.

Since the isolating capacity of the canister and the buffer might be threatened if deposition holes were positioned within a regional or local discontinuity, the geometric parameters are also of essential and indirect importance for this. Little precision is required in the data, however, provided it can be guaranteed that the discontinuities are located at a sufficient distance from the deposition holes.

Several parameters are of indirect importance for the mechanical stability of the rock. This is true of information on movements (size, direction and age) as well as the properties of the discontinuities for those fractures that are "included in" the discontinuity. Of the latter, parameters such as number of fracture sets, spacing, block size, fracture roughness, fracture filling (fracture mineral), and alteration/weathering are all of essential but indirect importance, since they are utilized in empirical formulas for the strength of the rock mass (see Chap. 3). These parameters are thereby also of great importance for construction analysis and layout. It should also be noted that the properties of the discontinuity can vary both across and in the plane.

Some of the information on the internal properties of the major discontinuities is also indirectly of importance for the retention properties of the rock, since fracture filling and fracture mineral influence geochemistry and sorption properties (see Chaps. 6 and 7). But the information is of limited importance, since it is relatively more important to know the retention properties in the portion of the rock situated closest to the repository.

All parameters, including genetic type, are of essential importance for the geoscientific understanding of the site.

2.7.3 Local minor discontinuities

Local minor discontinuities do not influence the overall placement of the repository, owing to their limited size, but do influence its detailed layout and the degree of utilization of the rock for the repository. This notwithstanding, individual minor discontinuities can be important, not least for the groundwater flow (cf. NE-1 on Äspö, which in size lies between local and local minor discontinuities according to Table 2-2). Obviously, efforts should be made to identify all presumed important local minor discontinuities within the projected repository area. At the same time, it is obvious that the probability of finding discontinuities is a direct function of their size, and to some extent their character (see e.g. Santaló, 1976 or Andersson et al., 1984). This means that the local minor discontinuities within the projected repository area primarily need to be described stochastically, even if certain discontinuities are identified deterministically. (If deterministic information is available, it should naturally be utilized.)

Depending on their properties, local minor discontinuities may be of essential importance for strength and groundwater flow in the rock. Moreover, since they can occur within the repository area, they are of great importance for the performance of the repository. This means that the geometric description of position, orientation, length and width (which in this case is partially stochastic) is directly of essential importance for layout and construction analysis, of essential importance for being able to judge the isolating capacity of the rock (see Chap. 3), and of essential importance for being able to judge groundwater flow on a site scale (see Chap. 5). Just as for the major discontinuities, it is important to characterize the extent of these discontinuities beyond the repository area as well, at least far enough out so that their contact with major discontinuities is described (see above).

The geological characterization of the discontinuities should include information (stochastic and in relevant cases deterministic) on movements (size, direction, age), genetic type and properties such as number of fracture sets, spacing, block size, fracture roughness, fracture filling/fracture mineral and alteration/weathering. In the immediate repository area, the interior of the discontinuities, which after all consist of individual fractures, should be described in the same way as individual fractures (see 2.7.4).

Just as for the major discontinuities, several parameters are of indirect importance for the mechanical stability (isolating capacity) of the rock. This is true of information on movement as well as the properties of the discontinuities for the fractures that "make up" the discontinuity. Of the latter, parameters such as number of fracture sets, spacing, block size, fracture roughness, fracture filling, fracture mineral, alteration and weathering are all of essential but indirect importance, since they are utilized in empirical formulas for the strength of the rock mass (see Chap. 3). These parameters are thereby also of great importance for construction analysis and layout (see section 2.8). Information on fracture sets, spacing, block size and fracture filling or the equivalent that can be used in, for example, discrete network modelling is of limited to essential importance for groundwater flow in the repository area (see Chap. 5) and thereby also for retention.

Some of the information on the internal properties of the local minor discontinuities is also indirectly of importance for the retention properties of the rock, since fracture filling and fracture mineral influence groundwater chemistry and sorption properties (see Chaps. 6 and 7). The information is, however, more essential (than for the major discontinuities), since transport via groundwater flow in minor discontinuities will represent a large portion of nuclide transport from the repository to the biosphere (see e.g. SKB-91 or SKI SITE-94).

All parameters, including genetic type, are of essential importance for the geoscientific understanding of the site.

2.7.4 Individual fractures

During the site investigation stage there is no other option than to describe individual fractures stochastically. There are different stochastic geometric models, which is briefly described in SR-95 and RD&D-95. Different concepts have different parameterizations (see Geier and Dershowitz, 1992, Winberg, 1994, Gylling et al., 1994). Since there are different discrete models for parameterizing a fracture network and since there are furthermore other models (e.g. stochastic continuum, which only uses the information indirectly), it would be inappropriate to stipulate in detail how fractures should be characterized. Instead, data should be collected that permit interpretation with different stochastic models (see 2.7.5 below). Moreover, it is important to collect enough data to enable different models to be used.

The geological characterization of individual fractures should include information that permits a stochastic description of networks of fractures (e.g. frequency, size, orientation and contact pattern) and that describes the properties of the fractures such as fracture width (includes both aperture and affected wall rock), roughness, fracture filling (fracture mineral) and alteration/weathering. The information on the fracture network in the repository area is of essential importance for determination of mechanical stability (see Chap. 3), for the detailed groundwater flow (see Chap. 5) and thereby also for the retention properties of the rock (see Chap. 7). The information is of limited importance in the construction analysis. The principal fracture direction can (together with the rock stress conditions) influence the orientation of the deposition tunnels and is therefore of limited importance for the repository layout.

Roughness, fracture filling, alteration, weathering/fracture mineral are further of essential importance for assessment of mechanical stability in the repository area, since these parameters are included in empirical formulas for strength (see Chap. 3). Fracture width and fracture filling are in practice only of limited importance for groundwater flow (direct hydraulic tests are necessary, see Chap. 5). Chemical characterization of fracture filling, fracture mineral and wall rock are of limited importance for choice of retention parameters, but of essential importance for understanding the retention mechanisms in the rock (see also Chap. 7).

2.7.5 Measurement methods

Discontinuities are located (identified) by means of geological, geophysical and hydrological methods. Their exact position, orientation and characterization are determined by means of drilling and various logging methods and tests in the boreholes. Normally at least 2–3 boreholes are required for each discontinuity (depending on conditions and measurement methods used). Based on the level of ambition, it is also in principle possible to evaluate how many boreholes are needed to actually find all discontinuities down to a given size and importance. Hydraulic interference tests can also be used to verify a discontinuity, although they should chiefly be used to determine hydraulic properties.

When positioning boreholes, it should be borne in mind that they cannot be positioned solely to verify major discontinuities. As is evident from the above description, information on minor discontinuities and fractures in the repository area is, even if stochastic, as a rule of essential importance to be able to make judgements of mechanical stability, detailed groundwater flow and retention properties. Furthermore, the need to gather other information (hydraulic and hydrochemical) should also influence borehole positioning. An optimal utilization of boreholes should therefore be an important aspect of the continued planning of the site investigation programme.

A stochastic description of discontinuities, such as individual fractures, can be estimated from data on fracture length, fracture frequency and orientation as measured in surface investigations and boreholes. The estimates are burdened by uncertainties and are dependent on the assumed geometric model in the discrete model, on the size and orientation of the observation area, and on the actual size and orientation of the fractures (see e.g. Dverstorp and Andersson, 1989).

There are different ways to handle the bias that arises (see e.g. Dershowitz et al., 1995). In general, however, it can be said that in order to get good data, the observation area should not be too small, which requires a high degree of exposure or uncovering of the rock surface in soil-covered areas. It is important to include both long and short fractures (this provides an opportunity to try which fracture distribution model is best). It is also important not only to use standardized sampling methods (e.g. "scanline sampling") – with computer simulation it is possible to utilize all information on fractures gathered on an observation area of arbitrary shape. If it proves necessary to choose, it is probably better to opt for a large observation area than many small ones.

Even though the geological structure model should primarily be seen as a source of input data to hydrogeological and groundwater chemical modelling, the possibility of utilizing hydrogeological/hydrochemical information for verifying structures should not be disregarded.

Trace element analyses should be performed on samples of fracture fillings with associated wall rock and on reference samples of fresh, unaltered rock as mentioned above in connection with determination of the retention properties of the rock for the safety assessment. It is then of the utmost importance that analyses be available of equivalent substances in water that has run through the sampled fractures. This relationship must be clear so that the results can be interpreted in a meaningful way. To trace the influence of co-precipitation, particular attention should be given to calcite, iron(III) and manganese(IV) minerals. See further Chap. 7.

3 Rock mechanics - mechanical stability

3.1 Overview of parameters, methods and areas of application

Table 3-1 summarizes rock-mechanical parameters that may be used in a rock-mechanical analysis. The table also tries to show examples of how the parameters are determined and how they are used. The parameters in Table 3-1 are also found in the collected parameter table in Appendix A:2.

Table 3-1. Overview of rock-mechanical parameters.

Parameter	Method	Used for
Discontinuities		
Geometry for discontinuities and geological parameters	See geological model	To divide rock into different rock masses in rock-mechanical model and as input data to determination of mechanical properties of rock mass.
Mechanical properties, fractures in different rock masses		Discrete rock-mech. model, input data to deformation properties for rock mass.
Deformation properties in normal direction	Lab (drill core), "Generic"	
Deformation properties in shear direction	Lab (drill core), "Generic"	
Strength in shear (⊥ , C,	Lab (drill core), "Generic", Field,	
Fracture roughness, JRC, Compressive strength of fracture wall, JCS)	Lab (drill core), "Generic"	
Mechanical properties, intact rock in different rock masses		Discrete rock-mech. model, input data to deformation properties for rock mass.
Young's modulus (E-modulus)	Lab (drill core), "Generic"	
Poisson's number (v)	Lab (drill core), "Generic"	
Compressive strength	Lab (drill core), "Generic"	
Tensile strength	Lab (drill core), "Generic"	
Indentation index, DRI, wear index	Lab (drill core), "Generic"	Assess drillability.
Blastability	Lab (drill core), "Generic"	Assess blastability.
Mechanical properties for different rock masses		
Young's modulus (E-modulus)	Mapping drill core, "Generic"	Rock-mech. model.
Poisson's number (v)	Lab (drill core), "Generic"	Rock-mech. model.
Rock classification (RMR, Q) different systems	Drill cores	Determination of deformation and strength properties.
Dynamic propagation velocity, compression wave	Measurement in field	Model for dynamic analysis.
Dynamic propagation velocity, shear wave	Measurement in field	Model for dynamic analysis.
Strength	Mapping drill core, "Generic"	Rock-mech. model.
Density and thermal properties		
Density	Lab (drill core), "Generic"	Rock-mech. model.
Coeff. of thermal expansion	Lab (drill core), "Generic"	Rock-mech. model.
Thermal conductivity	Lab (drill core), "Generic"	Rock-mech. model.
Specific heat	Lab (drill core), "Generic"	Rock-mech. model.

cont'd. on next page

Parameter	Method	Used for
Boundary conditions and supporting data	Overcoring, hydraulic fracturing, "Generic", ...	Assessment stability, (calibration).
In situ stresses, magnitude and directions	Scenario analysis, buffer, ...	Rock-mech. model.
External loads		
Observed deformations and seismic activity	"Mapping", seismic observations	"Validation".

3.2 Models and areas of application

Mechanical stability is one of the bedrock's fundamental safety features (see e.g. supplement to RD&D-Programme 1992, SKB, 1994). Mechanical stability mainly entails that the performance of the buffer and the canister should not be compromised by movements in the rock, and that movements or new fractures may not essentially alter the groundwater flow around the repository in such a way that its retention properties are seriously impaired.

The evaluation of mechanical stability can be divided into different *scales* and different *time perspectives* for different *loads*:

- On a repository scale, the stability of the rock is analyzed as a consequence of, among other things, thermal changes, dynamic loads, as well as large-scale changes in the load situation (e.g. a glaciation).
- Mechanical stability on a tunnel or deposition hole scale needs to be evaluated in connection with construction analysis and operation, but is also essential for the long-term performance of the repository. After closure the effect of static load, resaturation and temperature changes needs to be analyzed, as does the influence of more large-scale changes in the load situation. Both construction aspects and long-term performance provide information on how deposition tunnels and deposition holes should be designed.
- Long-term mechanical impact on groundwater flow (mainly in the near field).

Figure 3-1 shows the structure and use of rock-mechanical modelling.

A general description of rock-mechanical modelling and questions surrounding it is provided in Hudson ed. (1993). Lejon (1993) goes through mechanical properties of fracture zones, with a special emphasis on questions of importance for final repositories. It can, however, be concluded that rock-mechanical questions have so far been given scant treatment in published safety assessments such as SKB 91 or SR 95. This also means that there is limited detailed experience of which rock-mechanical parameters are of importance for long-term safety, even though general knowledge exists about this.

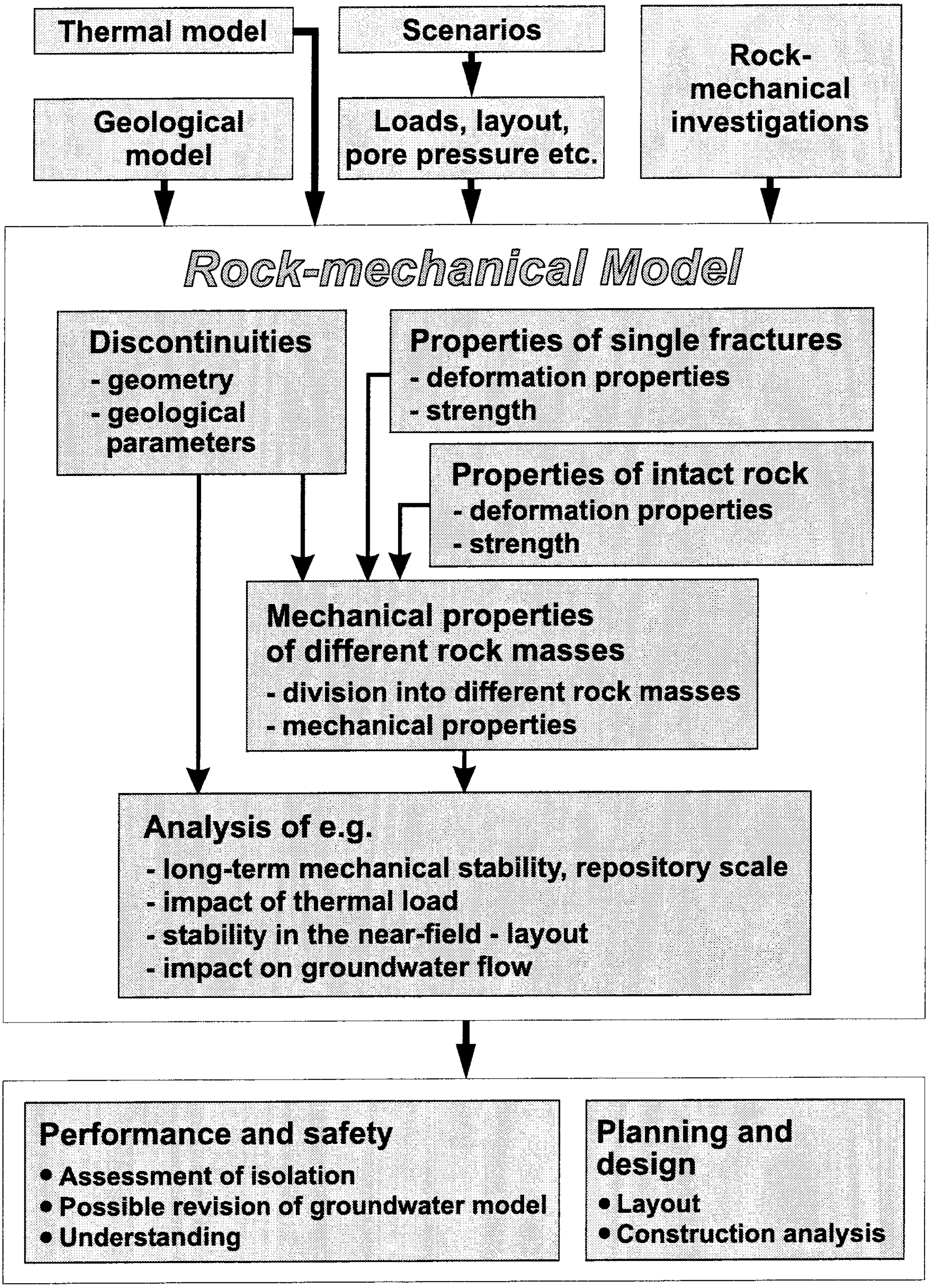


Figure 3-1. Schematic illustration of structure and use of rock-mechanical modelling.

3.2.1 Mechanical stability on repository scale and thermal load

An analysis of the long-term mechanical stability of the repository seeks to determine whether unacceptable movements or new discontinuities can arise as a result of the repository's geometry and the different loads to which the repository will be subjected. These loads include prevailing stress conditions, those that arise due to temperature changes, external loads such as an ice cap and dynamic loading from e.g. earthquakes.

The repository-scale analysis does not necessarily have to be done with quantitative models. Identification of large-scale deformation zones and determination of the general stress situation may be enough. In this case, the approach may be based more on generic quantitative analyses of the large-scale impact of heat, ice loads etc. However, the large-scale analysis needs to be able to provide boundary conditions for a rock-mechanical analysis on a near-field scale. Quantitative analysis has to be performed as a rule to ensure that thermal expansion does not cause any problems, such as tensile stresses that go down to excessive depths.

Quantitative rock-mechanical analysis (see e.g. Israelsson et al., 1992) can also be done using calculation programs where stresses and deformations are calculated for given external loads. In some models, the rock is described as being composed of discrete blocks bounded by discontinuities. In principle, different deformation and strength models can then be assigned to the discontinuities and the rock mass in the blocks. The rock can also be described as a continuum (with a finite element model). In this case, the modelled discontinuities and the rock are described with the same model, as a rock mass consisting of fractures and discontinuities, but the discontinuities are represented with other values of the deformation and strength parameters. As a rule, however, models contain *both* discretely represented elements and averaged information. The choice between these options is scale- and problem-dependent, as described for example by Lejon (1993).

3.2.2 Stability in the near field, design questions

Evaluation of stability in the near field and suitable design of deposition drifts and deposition holes pertain to performance in both the short and long term. A large number of analyses have been performed to determine how large deformations of deposition holes are required to damage the canister, but modelling work is still in progress (see e.g. Börgesson et al., 1995). These results can be used, together with the mechanical analyses for example, to arrive at criteria for acceptance of deposition tunnels and drifts, and to provide guidance for their orientation and design (e.g. assessment of reinforcing needs, and risk of rock burst problems), for assessment of the formation of an excavation-disturbed zone, and for input data to source term calculations. This means that questions regarding constructability, design and safety are strongly linked.

The evaluation should preferably be based on quantitative calculations. The modelling tools that are used are similar to those that can be used on a larger scale, but in order for modelling to be meaningful, discontinuities need to be described with a higher degree of detail. Based on data from a site investigation, fractures and deformation properties can only be described stochastically (equivalent problems as for groundwater flow) and are therefore as a rule described as a rock mass (or in principle with simulation of different fracture geometries). The fracture information on a near-field scale can be supplemented in conjunction with detailed characterization and repository construction.

3.2.3 Assessment of hydromechanical couplings

Rock-mechanical changes affect the rock's conductivity (hydromechanical influence). Modelling of hydromechanical couplings is of a research character and is one of the central themes in the DECOVALEX project (see e.g. Jing et al., 1993). In other words, the importance of hydromechanical couplings may need to be included in a safety report on a site.

3.2.4 Favourable, unfavourable and discriminating factors

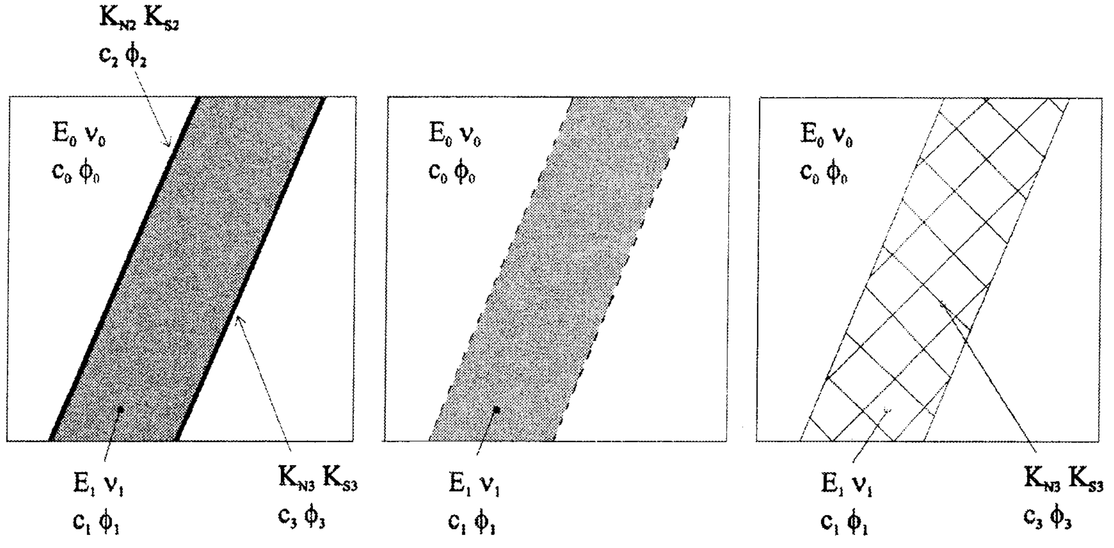
In the supplement to RD&D-Programme 92, a number of rock-mechanical factors are rated as favourable, unfavourable or discriminating.

The following were rated as *favourable* factors: rock stresses and thermal conductivity properties normal for Swedish bedrock, homogeneous and easy-to-interpret bedrock and access to rock blocks with few fracture zones and low fracture frequency surrounded by clear zones of weakness, i.e. very similar to the factors mentioned under geology. The following were rated as *unfavourable* factors: anomalous rock stress conditions, anomalous strength properties, strongly heterogeneous and difficult-to-interpret bedrock, nearness to known deformation zones and postglacial faults. Factors rated as *discriminating* in the sense that they can occasion abandonment of a site where site investigation has begun were: extreme rock-mechanical properties. This factor obviously needs to be defined more precisely to be directly usable, but an important example may be high rock stresses in relation to the strength of the intact rock.

The identification of rock-mechanical parameters in the following sections covers all the parameters mentioned above. A further definition and possible revaluation of site selection factors based on the rock-mechanical model can, in other words, be based on the list of parameters in Appendix A:2.

3.3 Discontinuities

The occurrence of discontinuities is very important in rock-mechanical modelling. They have arisen due to mechanical action and have other deformation properties than the intact rock. The deformation properties of the major discontinuities are dependent on the deformation properties of the intact rock, on the deformation properties of the fractures that make up the discontinuity, and on the geometry of these fractures. By *intact rock* is meant in rock-mechanical contexts *rock without visible fractures.*



Model with discrete fracture elements in contact with wall rock

Model without discrete fracture elements

Model with discrete rock blocks and discrete fracture elements

Figure 3-2. Different models for describing the mechanical properties of the rock mass in different discontinuities. For further information on the parameters in the figure, see Lejon, 1993.

In connection with practical rock-mechanical modelling of stability on a repository scale, only the major discontinuities are modelled explicitly, and then as a rule as zones with deviant deformation properties. The rock, both in fracture zones and in between, is denoted by the term *rock mass*, which represents the deformation properties for fractures and intact rock together.

Information on discontinuities is used to divide the rock into different rock masses in a rock-mechanical model. Discontinuities that are judged to be mechanically essential are described as rock masses with different mechanical properties. The rock between the explicitly modelled discontinuities is described as a rock mass with other mechanical properties. As is evident from Figure 3-2, different models can be used to describe the mechanical properties of the rock mass in different discontinuities.

Necessary parameters are therefore geometry of modelled discontinuities such as position, orientation and width, deformation and strength properties of the rock mass in the discontinuities, and deformation and strength properties of the rock mass between the modelled discontinuities.

In connection with the modelling of stability in the near field, individual fractures can also be modelled. The rock mass between the modelled fractures can consist of intact rock in a detailed model. In this case properties corresponding to the intact rock are chosen. If there are also fractures in the rock mass between the modelled fractures, the properties of the rock mass must be chosen with reference to the geometry and properties of these fractures and the properties of the intact rock.

Necessary parameters are geometry of modelled fractures, deformation properties and strength of these fractures, and properties of the rock mass between the modelled fractures.

Evaluation, need for resolution and measurement methods

To identify areas on the site that will be mechanically stable in the long term, it is necessary at least to identify all regional and major local discontinuities. Properties of the rock mass in the modelled discontinuities and other rock need to be determined. In principle, all parameters are equally important. In a given model and a special analysis, one parameter may turn out to be of greater importance than others, but this is difficult to determine in advance before the analysis has been performed. It is therefore stated in the summarizing table in Appendix A:2 that the geometric information is of essential importance for the isolating capacity of the rock and thereby of essential importance for the isolating capacity of the bentonite and the canister, of essential importance for the groundwater flow, and of essential importance for layout and construction analysis. (Windelhed and Alestam (1996) say that there is a need to identify discontinuities and make a rock-mechanical and stability assessment for them.)

Geometric information on the discontinuities is obtained from the geological structural model. The properties of the rock mass cannot be measured directly, but are estimated using different assumptions obtained from knowledge and measurement of mechanical properties of fractures, mechanical properties of intact rock, plus knowledge of fracture geometry. The following sections (3.4 – 3.6) describe these parameters in greater detail.

3.4 Mechanical properties of fractures in different rock masses

The mechanical properties of different rock masses are determined to a large extent by the mechanical properties of the fractures contained in them. The mechanical properties of fractures are dependent on their waviness, surface roughness, the strength of surrounding rock, fracture-filling material and degree of filling.

Rock-mechanical modelling should also take into account the water pressure in the fractures, since this influences the effective stress. In many practical cases, this influence is small in comparison with prevailing uncertainties, but the effect should be taken into account in connection with resaturation of the repository and at the very high water pressures that could conceivably arise during a glaciation.

3.4.1 Deformation properties

When a fracture is subjected to a purely normal load, it is pressed together until it has closed entirely. The relationship between normal stress and normal deformation is usually designated with the aid of normal stiffness, K_n, as long as the normal deformation is less than the fracture's maximum compression. The normal stiffness is dependent on the normal stress. Test loadings show that the relationship between normal stress and normal deformation can be approximated with a hyperbola.

In the same way as in the normal direction, the shear movements that occur in the shear direction prior to fracture can be designated with the aid of a shear stiffness, K_s. The size of the shear stiffness is also stress-dependent.

3.4.2 Strength

The shear strength between two plane surfaces can be described with a base friction angle. The natural fractures are never so plane that the shear strength of the fractures is determined by the base friction angle. Generally, fracture roughness increases strength. The shear strength of a saw-toothed fracture is dependent on the base friction angle between two plane surfaces (ϕ_b) and the angle of the saw tooth i, provided normal stresses are low when sliding takes place along the asperities. At high normal pressures, asperities are sheared off from the intact rock and the shear strength is dependent on the strength of the intact rock.

Barton (1973, 1976), Barton and Chonbey (1977) and Barton and Bandis (1990) have studied the behaviour of rock fractures (joints) and proposed formulas based on the roughness coefficient of the fracture (Joint Roughness Coefficient, JRC) and the compressive strength of the fracture wall (Joint Compressive Strength, JCS). Both parameters are scale-dependent and can be determined both in the field and in the laboratory. The determination is made on a reference length of 100 mm.

3.4.3 Evaluation, measurement methods and requirements on precision

In principle, all parameters are equally important. In a given model and a special analysis, one parameter may turn out to be of greater importance than others, but this is difficult to determine in advance before the analysis has been performed. It is therefore stated in the table in Appendix A:2 that all of the above-mentioned parameters are of essential importance for isolation (rock, bentonite and canister) and essential importance for design (layout and construction analysis). Deformation properties and strength are of limited importance for the groundwater flow, since they determine the importance of hydromechanical couplings.

The deformation and strength properties of the fracture can be determined by testing in a shear box in the laboratory or in the field. The tests are conducted on relatively small-scale samples, which means that the test result must be scaled up to actual fracture lengths.

To be able to use Barton's relationship, JRC and JCS are determined by mapping in the field and on retrieved core samples.

The requirement on precision in determination of the deformation and strength properties of fractures is dependent on the problem to be analyzed, and no general guidelines can be given. To determine this requirement more exactly, a sensitivity analysis must be carried out for the specific problem.

3.5 Mechanical properties for intact rock in different rock masses

The mechanical properties of different rock masses are also determined by the mechanical properties of the intact rock contained in a particular rock mass. (By *intact rock* is meant, as mentioned above, in rock-mechanical contexts *rock without visible fractures*.) The central rock-mechanical data pertain to the constitutive relationship between stress and strain. Since intact rock is a brittle material, the choice of material model is not given. Among other things, it can be discussed whether creep, failure criterion and hysteresis are handled correctly in the models used today. This question is not, however, solved by a site investigation programme – "generic" information and research are needed to get further, if this should be deemed necessary.

As a rule, the mechanical properties of the intact rock are described with a linear portion and a plastic portion which is dependent on the strength of the material.

3.5.1 Deformation properties

The linear portion is described with elasticity theory in the form of the modulus of elasticity (Young's modulus) and Poisson's number. Both parameters are determined from test loading of drill cores. The modulus of elasticity is generally dependent on the surrounding load ("restraint") and the "microfractures" in the rock.

3.5.2 Strength

The plastic portion is usually described with a flow function and a flow rule. The flow function, F, is dependent on the stresses and encloses a volume in the stress space within which stress changes give rise to purely elastic strains. Stress changes outside of the flow surface give rise to plastic strains. The flow potential, Q, describes how the plastic strains take place.

A widely used model for the plastic portion is Mohr-Coloumb's model where the flow function, F, is described with a cohesion, c, and an inner friction angle, ϕ, and where the flow potential, Q, is described with the aid of a dilatancy angle, Ψ.

There are specially developed material models for rock material, e.g. Hoek and Brown's failure criterion (Hoek and Brown, 1980). The failure criterion includes two material parameters, namely the uniaxial compressive strength of the intact rock, σ_c, and a constant, m_i, which is dependent on the properties of the rock. The uniaxial compressive strength, σ_c, should be determined by laboratory testing of drill cores with a diameter of 50 mm and a length of 100 mm, but can also be estimated from σ_{cd}, which is the uniaxial compressive strength measured on a specimen with a diameter of d mm.

The parameters for Mohr-Coulomb's and Hoek and Brown's failure criterion are determined from triaxial loading tests to failure carried out at different lateral pressure on drill cores.

To be able to study how the intact rock behaves during and after failure, the tests should be performed in a rigid, deformation-controlled press. Behaviour after failure is of importance when the risk of rock burst is to be judged.

There are no clear-cut relationships between rock type and strength; instead, there is great variation. There is, however, less variation in strength for a rock type within the same pluton.

3.5.3 Evaluation, measurement methods and requirements on precision

In principle, all parameters are equally important. In a given model and a special analysis, one parameter may turn out to be of greater importance than others, but this is difficult to determine in advance before the analysis has been performed. It is therefore stated in the table in Appendix A:2 that all of the above-mentioned parameters are of essential importance for isolation (rock, bentonite and canister) and essential importance for design (layout and construction analysis). The parameters are of limited importance for groundwater flow, since they determine the importance of hydromechanical couplings. Strength is, however, of essential importance for groundwater flow, since new flow paths could be created.

Measurement methods have already been commented on above. Requirements on precision are problem-dependent.

3.5.4 Indentation index, wear index and blastability

It is stated in Windelhed and Alestam (1996) that indentation index, DRI and wear index, as well as blastability, are needed for planning and design of the rock works. These parameters have been given the assessment L for layout and E for construction analysis in the collected parameter table (A:2).

3.6 Mechanical properties for different rock masses

The properties of the individual fractures and the intact rock blocks determine the behaviour of the different rock masses. Depending on the geometric distribution of fractures, the rock mass will behave isotropically or anisotropically. The more fractures with different directions intersect the rock mass, the more isotropic their behaviour will be. To determine the mechanical properties of the rock mass, parameters are thereby needed that describe the geometry and properties of the fractures. Examples of such parameters are those that occur in the empirical Q and RMR systems.

3.6.1 Deformation properties

The deformation modulus of the rock mass is lower than that of the intact rock. The deformation modulus can be obtained by adding together the contributions from the fractures and the rock blocks. The resulting modulus will be a function of the properties of the fractures and the rock blocks plus the distance between the fractures.

Another way to estimate the deformation modulus of the rock mass is to use empirical relationships based on a classification of the rock mass according to the Q or RMR system.

Poisson's number for the rock mass is estimated on the basis of Poisson's number for the intact rock and the geometry and properties of the fracture sets. Poisson's number for a rock mass varies between 0.2 and 0.3.

Knowledge of the deformation properties of the rock mass under dynamic loading is required for dynamic analyses. These are evaluated from the propagation velocity of compression and shear waves.

Evaluation, measurement methods and requirements on precision

The deformation properties of a rock mass are important parameters in all types of numerical modelling. The table in Appendix A:2 therefore rates these parameters as being of essential importance for isolation (rock, bentonite and canister) and of essential importance for design (layout and construction analysis). The parameters are of limited importance for the groundwater flow, since they determine the importance of hydromechanical couplings. The rock classification (in the form of Q or RMR) is an empirical parameter but is of essential importance in practice for the isolating properties of the rock. The dynamic deformation properties are of essential importance for isolation (rock, bentonite, canister), but are scarcely essential during a construction phase.

Direct determination of the deformation modulus in the field is difficult and costly. The empirical relationships developed to estimate the deformation modulus based on the rock mass according to the Q or RMR system are therefore normally used.

The dynamic properties are determined from field measurements, seismic methods, cross-hole measurements etc. where the propagation velocity for a compression or shear wave is determined.

The requirement on precision in determination of the deformation properties of the rock mass is dependent on the problem to be analyzed, and no general guidelines can be given. To determine this requirement more exactly, a sensitivity analysis must be carried out for the specific problem.

3.6.2 Strength

In many load cases, the strength of a rock mass intersected by three or more fracture sets is dependent for the most part on the properties of the fractures. Strength varies in these cases only to a small degree with the loading direction.

The Mohr-Coulomb failure criterion can be used to describe the strength of the rock mass within a limited stress range. There are different empirical relationships between classification of the rock mass according to the Q or RMR system and the included parameters c and ϕ.

The Hoek and Brown failure criterion has also been developed to describe the strength of a rock mass (Hoek et al., 1995). The component parameters are the value of the constant m for the rock mass (m_b), constants that depend on the character of the rock mass (s and a), and the uniaxial compressive strength of the intact rock (ϕ_c). The component parameters m_b, s and a, which describe the character of the rock mass, can be estimated with the aid of rock mass classification according to the RMR or Q system.

Evaluation, measurement methods and requirements on precision

The strength of the rock mass is obviously of essential importance for isolation (rock, bentonite, canister) and of essential importance for design (layout and construction analysis). Indirectly, strength is of essential importance for groundwater flow, since new flow paths could arise. The evaluation is shown in Appendix A:2.

Direct determination of the strength of the rock mass in the field is difficult and costly, since it requires loading of a large volume. The empirical relationships that have been developed to estimate the strength of the rock mass based on its classification according to the Q or RMR system are therefore normally used.

The requirement on precision in determination of the strength properties of the rock mass is dependent on the problem to be analyzed, i.e. how sensitive the result of the analysis is to variation in the strength of the rock mass. This sensitivity must be determined by a sensitivity analysis when the analysis is carried out.

3.7 Density and thermal properties

Thermal expansion, thermal conductivity and specific heat etc. are included as modelling data in calculating the stress changes and deformations that occur due to thermal loading. In such calculations, the component parameters are obviously of essential importance for the isolating capacity of the rock, as well as for the layout of the repository (see the table in Appendix A:2).

Generic data can be used (based on previous laboratory measurements) in combination with determinations made on drill cores from the specific site. The value of the parameters varies with the composition of the rock, particularly the quartz content. For further discussion of thermal properties, see Chap. 4.

3.8 Boundary conditions and supporting data

3.8.1 Rock stresses

The rock mass is subjected to stresses depending on the weight of the overburden and loads of tectonic origin. When a rock chamber or tunnel is excavated, a redistribution of stresses takes place locally and a local state of stress is created around the opening. Knowledge of the size and direction of these in-situ and induced stresses is a central part of the design of a rock facility. The rock stresses are thus an important input parameter for all types of modelling of mechanical stability on different scales, and for assessment of mechanical long-term stability, as well as in hydromechanically coupled calculations.

The regional stress field is applied as a boundary conditions for the regional rock-mechanical model. It is common for the calculation model to be oriented so that only normal stresses need to be taken into account along the boundaries of the model.

The stress field is also an important supporting parameter. The rock-mechanical models calculate the stress distribution in the rock around an opening, for example. If the stress field were instead known, it could be determined directly whether there was a risk of new fracture formation or other dramatic deformations. A measured stress field around e.g. an opening could also be used to verify the plausibility of calculation results.

Evaluation, measurement methods and need for precision

As is evident from the above discussion, and shown in Appendix A:2, information on stress distribution is of essential importance for isolation (rock, bentonite, canister) and design (layout and construction analysis).

Data on the regional stress field is taken from "generic knowledge". Rock stress maps can be obtained where the main directions of the in-situ stress field are shown (see e.g. Larsson and Tullborg, 1994 and Ljungren and Persson, 1995). These data must be augmented with geological information and rock stress measurements on the specific site. Regional structures in the rock mass may have rotated the in-situ stress field.

The main purpose of the rock stress measurements is to obtain a general picture of the rock stress conditions as regards magnitude and direction in the area, and an idea of conditions at block level. The need for precision is largely dependent on the strength of the rock mass and the sensitivity of the structure to variation in in-situ stress fields, above all the geometric configuration of the opening.

Measurement can be carried out by overcoring or hydraulic fracturing. The measurement is performed in boreholes. The advantage of hydraulic fracturing is that the measurements can be performed in already drilled holes, while determination by overcoring is done in connection with drilling. However, determination by overcoring yields better information on orientation compared with hydraulic fracturing.

During coring, indications of high rock stresses in relation to the strength of the rock can be observed in the form of "core discing". In all types of boreholes, "breakouts" can also be observed at very high stresses. The location of these breakouts around the periphery of the borehole gives an indication of the direction of the stress field.

There are several uncertainties involved in the determination of site-specific stresses, and furthermore the stress field varies in space, even over very short distances. It can be discussed whether a large part of the variation is due to a combination of measuring error and residual stresses inside the block. Satisfactory estimation of the local stress field requires relatively many determinations, and statistical treatment of the results. Uncertainties in stresses are, however, judged to be lower than uncertainties in the determination of strength and deformation properties. Stress determinations are therefore important.

3.8.2 Loads

Loads are used as boundary conditions in rock-mechanical calculations. They can be divided into loads from the repository and loads on the rock mass as a whole. The former (heat output, excavation of tunnels, swelling pressure etc.) are well known and are not site-specific (but are design-specific!!).

Loads on the rock mass as a whole comprise the regional stress field (see above) and future loads connected with scenarios such as glaciation, permafrost, earthquakes etc. Knowledge of these is essentially generic (see e.g. Boulton and Payne 1993 or King-Clayton et al., 1995). Regional differences exist, but there is hardly anything that can or needs to be measured.

Information on changes in external loads is of essential importance for isolation (rock, bentonite, canister) and of essential importance for groundwater flow. But the information is of minor importance for design under present-day conditions.

3.8.3 Identified deformations and seismic activity

Geological information can be crucial for determination of the long-term mechanical stability of the rock and the repository. Geological evidence for deformation zones and postglacial faults (or the absence of same) is important background information (see e.g. Stanfors and Ericsson, 1993). In published safety assessments (SKB 91, TVO-92), it is even argued that future displacements in the rock are directly linked to the size of present-day discontinuities. However, such arguments would have to be refined before they can be used as a point of departure for target specification of a site investigation. The geological model that is described in Chapter 2 ought to be a reasonable point of departure for a rock-mechanical assessment, and data requirements stipulated there take this into account.

4 Thermal properties

4.1 Overview of parameters, methods and areas of application

Table 4-1 summarizes which data are primarily needed to be able to describe the thermal properties of the rock. The parameters are also shown in the collected parameter list in Appendix A:3.

Table 4-1. Overview of data requirements for being able to determine the thermal properties of the rock.

Parameter	Method	Used for
Thermal properties of rock		Design, thermal modelling, rock mechanics.
Thermal conductivity – rock	Generic – test on drill core	
Heat capacity – rock	Generic – test on drill core	
Thermal expansion	Generic – test on drill core	
Temperatures		Modelling, design.
Temperature in rock and groundwater	Temperature measurement in borehole	Initial data for modelling.
Thermal boundary conditions/ gradient	Generic – temperature measurement	Boundary conditions.

4.2 Models and areas of application

Temperature and temperature distribution are fundamental condition parameters in the deep repository. The temperature influences the mechanical environment, the groundwater flow and the chemical/biological environment, although the influence is relatively moderate within the temperature range normally considered to prevail in the deep repository. Temperature conditions directly affect the layout and design of the repository. Figure 4-1 illustrates schematically the structure and use of thermal models.

4.2.1 Modelling of thermal evolution

Calculation of the thermal evolution is described in section 10.2 in SR 95. Heat is transported by heat conduction. The spent fuel is a heat source. Simple geometries are treated analytically. Numerical solution methods (the FEM models ANSYS and SOLVIA) are used in more complicated cases.

Besides via conduction, heat can also be transported advectively with the flowing groundwater. At high porosities, advection with the flowing water is significant and cannot be neglected. However, several studies (e.g. Thunvik and Braester,

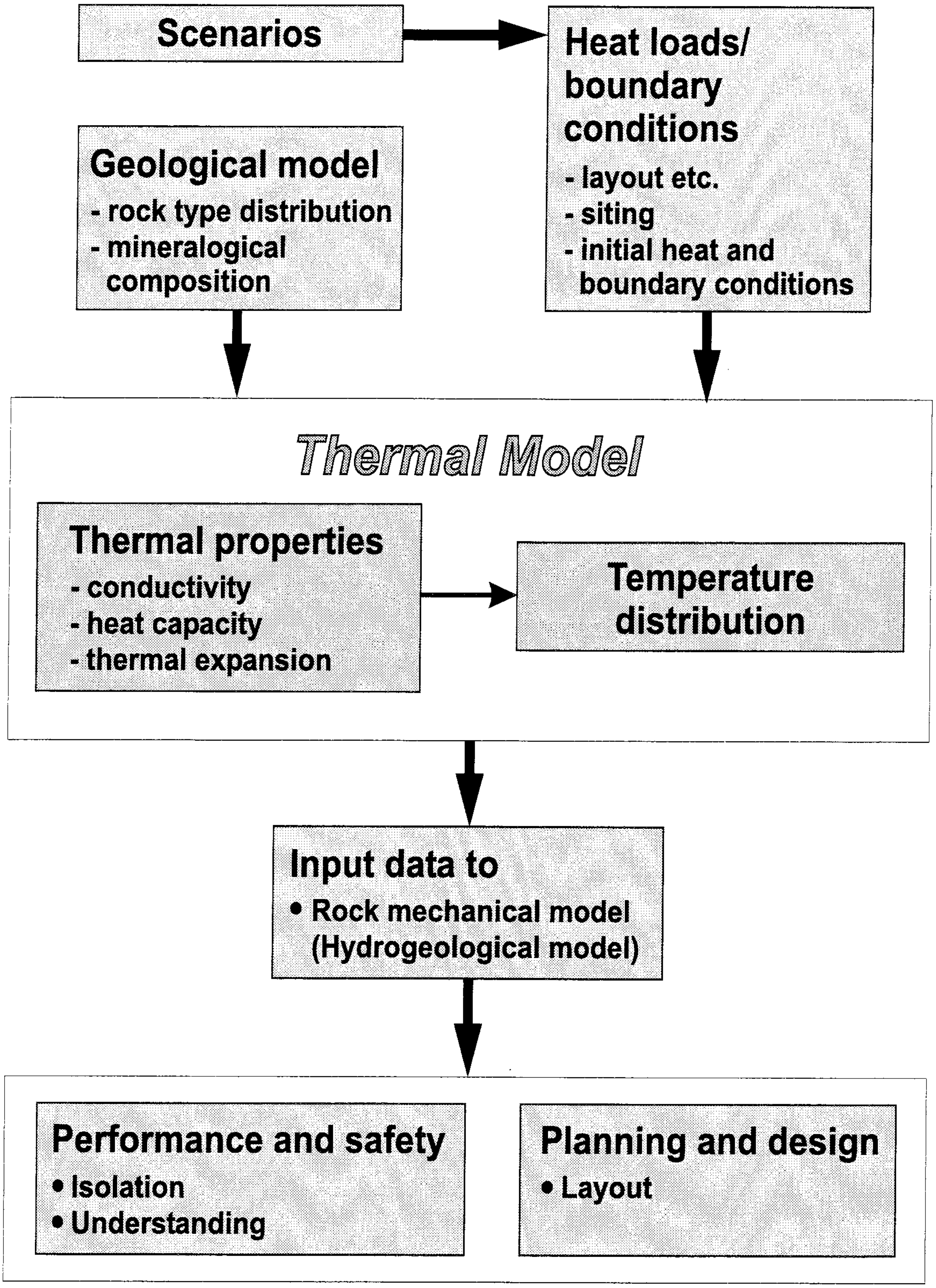


Figure 4-1. Schematic illustration of structure and use of thermal models.

1980) show that heat conduction is the predominant transport mechanism in fractured rock. Porosity, which lies between 10^{-3} and 10^{-4}, is so low that the heat content of the groundwater can be neglected.

Heat transport is determined by the conductivity, density and heat capacity of the rock mass. These properties vary in space, but this variation is moderate on a large scale. This spatial variation could conceivably cause problems on a near-field scale, however.

Conceivable heat sources are in principle well known. The residual (decay) heat from the spent fuel derives from radioactive decay and can therefore be calculated. The heat output of individual canisters is dependent on the composition of the spent fuel and the interim storage period, i.e. the chosen strategy for encapsulation and management of encapsulated fuel. In principle, individual variations between canisters should be able to be calculated or measured.

Small variations in climate have very little influence on the temperature at great depths. During long periods of permafrost, the upper parts of the rock freeze. The exact depth of the permafrost is difficult to estimate, but even simple calculations are sufficient to show that it doesn't reach repository depth.

4.2.2 Mechanic, hydrological and chemical impact of temperature

The temperature increase and subsequent cooling in the repository cause, via the thermal volume change of the rock, relatively substantial stress redistributions in the rock in and around the repository area. Once the repository is completed, the temperature load is the most important mechanical force acting on the repository until such dramatic climate-driven events as permafrost and glaciation.

Groundwater movements are affected by the thermal gradient that arises, but also by potential changes in the rock's fracture structure. As is noted in Chapter 5 (hydrogeology), however, the driving force from the thermal density differences is often negligible in comparison with other driving forces (e.g. topography). Nevertheless, the importance of the thermal gradient has to be evaluated for each individual case, even though complicated coupled groundwater calculations can usually be avoided.

Temperature is an important parameter in most chemical, biological and physical processes and thereby affects e.g. equilibria (solubilities) and kinetics. Microbiological activity is also highly temperature-dependent. The influence of temperature changes is relatively moderate within the temperature ranges normally believed to prevail in the final repository. It is possible within a relatively large temperature range to conservatively choose suitable chemical parameters that are temperature-independent within the range. The thermal analysis must, however, show that the temperature does not become excessively high (e.g. higher than 100°C) or excessively low. Essential changes can occur at the extreme temperatures, but these are preferably not analyzed due to inadequate knowledge, and it is easier to make sure that these extreme temperatures will not occur at repository depth.

4.2.3 Design and layout

The heat output of individual canisters is dependent on, among other things, the quantity and composition of the spent fuel and the interim storage period, i.e. the chosen strategy for encapsulation and management of encapsulated fuel, and the temperature of the repository is dependent on how densely canisters are emplaced in it. In principle, it is desirable to pack the spent fuel as tightly as possible, without excessively high temperatures arising. The conditions for heat transport in the deep repository are therefore important in connection with repository design and layout. SR 95 also states that "...studies of the heat transport in and around the deep repository comprise an important element in both safety assessments and repository design and layout. They have therefore been included in the development work for the deep repository right from the start."

4.2.4 Favourable, unfavourable and discriminating factors

In the supplement to RD&D-Programme 92, heat conduction properties that are normal for Swedish bedrock are rated as *favourable* thermal conditions. It can however be discussed whether this is really favourable and not merely acceptable. *Unfavourable* or *discriminating* factors are not defined, aside from what can be covered by the phrase "strongly heterogeneous and difficult-to-interpret bedrock", which has already been taken up in the geology chapter. As for other conditions, it may be a good idea to evaluate whether other unfavourable or discriminating factors might exist, such as for example many mineral boundaries with low/high thermal conductivity (could result in undesirable fracturing), or potential hydrothermal reservoirs (risk of intrusion). A further definition and possible revaluation of site selection factors can be based on the list of parameters in Appendix A:3.

4.3 Parameters

Information on the thermal conductivity and heat capacity of the rock as well as on current temperatures in rock/groundwater and the thermal gradient are needed to determine the temperature distribution in the rock under different conditions.

4.3.1 Thermal properties of the rock

Heat transport through the rock takes place via conduction. This is determined by heat capacity and thermal conductivity. Both of these parameters are of essential importance for layout, as well as for the isolating capacity of the rock (canister, bentonite, rock) via thermomechanical effects. Heat transport directly influences the conditions for thermally driven groundwater flow, but since as a rule this is subordinate to other driving forces heat transport will be of limited importance for groundwater flow. The importance of the coefficient of thermal expansion has already been discussed in the chapter on rock-mechanical parameters (Chap. 3).

It should be most important to have a good lithology model to be able to carry out thermal calculations. Coefficient of thermal conductivity and specific heat capacity can be derived in an acceptable fashion from mineral composition. The distribution of different minerals, especially on the near-field scale, needs to be taken into account. The importance of mineral boundaries within a deposition hole may have to be analyzed in special performance studies.

The thermal properties of the water in the rock (thermal conductivity and specific heat), as well as how the water is affected by temperature changes (viscosity and density), are well known from the literature (see e.g. Bird et al., 1960) and do not have to be determined site-specifically. Furthermore, the water can as a rule be neglected when calculating heat transport in crystalline rock, since porosity is so low that only a very small fraction of the heat energy can be stored in the water.

4.3.2 Temperatures

The temperature distribution at depth shows considerable regional variation, from about 20°C in the south to about 8°C in the north. The original temperature is of essential importance for repository layout, since it is one of the determining factors for what canister density can be accepted and is needed as an initial criterion in modelling of thermal evolution. Site-specifically measured temperatures can be important for confirming assumed parameters and are important for the geoscientific understanding of a site. Temperature has a limited influence on groundwater flow and chemistry and is therefore of limited importance for these aspects.

The temperature boundary conditions are essential for the thermal modelling and thereby indirectly for the aspects already discussed. At depth, the boundary conditions are determined by the geothermal gradient. This can also be important for assessment of the risk of intrusion due to the presence of geothermal reservoirs. On the surface, the temperature boundary conditions are determined by the annual mean temperature, which exhibits regional differences. In the long time perspective, climatic variations will arise, where permafrost in particular could have a relatively great impact (see e.g. King-Clayton et al., 1995), and it is then important to demonstrate that permafrost does not reach repository depth.

5 Hydrogeology

5.1 Overview of parameters, methods and areas of application

Table 5-1 summarizes which data are primarily necessary to be able to construct the different hydrogeological models that are needed. The table also attempts to show examples of what measurements can be used to estimate the parameters and how they are used. The parameters in Table 5-1 are also shown in the collected parameter table in Appendix A:4.

Table 5-1. Overview of data requirements for description of hydrogeology, measurement methods and areas of application. See text for further explanation.

Parameter	Method	Used for
Deterministically modelled discontinuities		
Geometry – see geological model	See geological model	Input data to models on site scale.
Permeability distribution	Hydraulic tests in and between boreholes	Input data to models on site scale.
Porosity	Lab test drill core/ Tracer test	Transient model.
Stochastically modelled discontinuities and fractures as well as rock mass		
Stochastic description of discontinuities	See geological model	DFN models, SC indirect on repository scale.
Permeability distribution	Hydraulic tests in and between boreholes – Extrapolation	Model data.
Porosity and Storage coefficient	Pumping test, extra-polation	Transient model.
Compressibility of rock	Generic/Measurements on drill cores	THM model.
Hydraulic properties of groundwater		
Salinity	Water tests	Model data/calibration.
Temperature	Borehole/Experience	Model data – certain.
Soil layers etc.		Groundwater models for Land and environment, Biosphere models, Interpret boundary conditions for groundwater models in repository area.
Identification of receptors	Hydro(geo)logical mapping	
Meteorological and hydrological data	Hydro(geo)logical mapping	
Conductivity, thickness, storage coefficient, etc.	Pumping test, layer sequences etc.	

cont'd. on next page

Parameter	Method	Used for
Boundary conditions and supporting data		
Regional boundary conditions, historical and future development	Climate modelling, Topography	Paleohydrogeology, Analysis of scenarios,
Pressure or head distribution	Topography, Boreholes (see text), large-scale model	Boundary conditions/ calibration.
Recharge/discharge areas	Mapping	Calibration, Receptor model.
Breakthrough curves	Large-scale tracer tests	Calibration.
Groundwater flow boreholes	Dilution probe etc.	Calibration.

5.2 Models and areas of application

Hydrogeological models have several areas of application in safety assessment and activities supporting safety assessment. A hydrogeological understanding also needs to be built up to explain long-term geochemical changes and coupled hydraulic and rock-mechanical phenomena. These applications are tied to different scales, and the need for input data differs slightly for these needs. In brief, models are used (or can be used) for:

- hydrogeological understanding, boundary conditions for detailed models, predictions of large-scale changes in groundwater chemistry etc.,
- predictions of inflow during the construction period, and resaturation after closure,
- input data to migration models (see Chapter 7),
- input data (flow) to near-field models (near-field flows),
- input data to biosphere models,
- evaluation of (other) near-surface environmental consequences (land and environment).

The hydrogeological analyses are coupled, as is illustrated schematically by Figure 5-1.

5.2.1 Hydrogeological understanding, boundary conditions and regional changes

Models for hydrogeological understanding and groundwater flux do not need to describe the flow pattern in the rock in detail. It is, however, important to determine realistic boundary conditions and ascertain the principal flow pattern. Such models can also be used to determine boundary conditions for modelling on a smaller scale. Experience indicates that large-scale flow can be described quite well with porous media models (e.g. NAMMU, which SKB uses). Regional

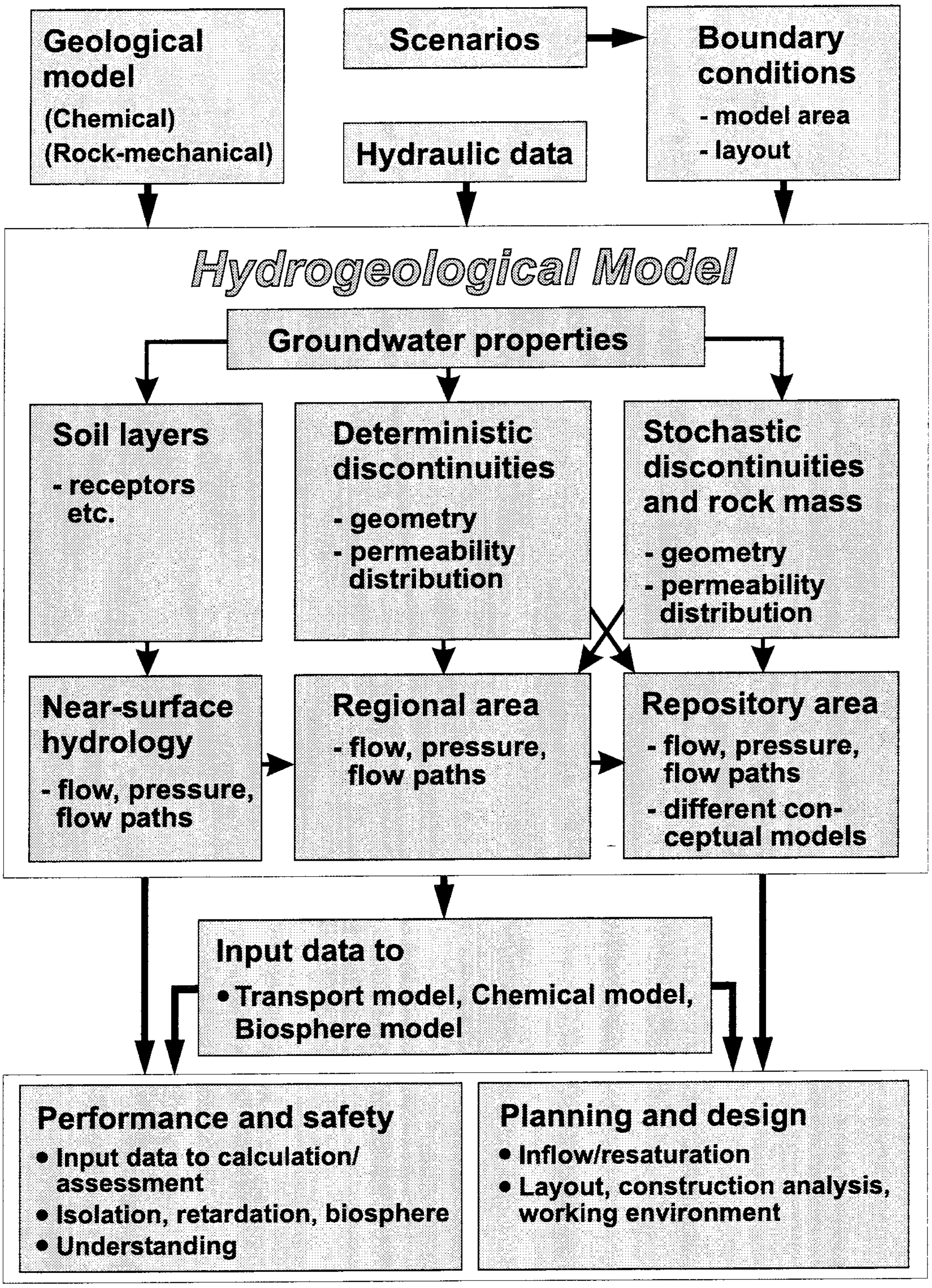


Figure 5-1. Schematic illustration of structure and use of hydrogeological models.

structures with deviant permeability need to be taken into account, even though the requirement on precision in knowledge of properties is limited compared with the needs in modelling of radionuclide transport. If the topographically influenced groundwater gradient is sufficiently large, it is possible to neglect thermal convection (Thunvik and Braester, 1980). Salinity and density effects coupled with changeable boundary conditions may have to be considered, however (Voss and Andersson, 1993, Follin, 1995).

5.2.2 Inflow during construction period and resaturation

Only a few studies (e.g. Follin, 1995) have analyzed groundwater flow in connection with resaturation after closure. Inflow and groundwater flow during the construction of the Äspö tunnel have, however, been analyzed (see e.g. Mészáros, 1996). Such studies may be given greater weight because they are linked to constructability (what size of water inflows may occur), but also to long-term safety, since the course of resaturation can decide the groundwater chemistry environment during the post-closure period.

In Follin's work, the fact that unsaturated groundwater flow can arise during the drainage period was taken into account. But it is not clear that it is necessary to take into account this complication. In principle, the shape of the "cone of depression" influences the size of the inflow. However, experience from Stripa shows that most of the rock mass is nevertheless water-saturated (Olsson ed., 1992). Both Follin and Mészáros also conclude, both from model results and comparison with Äspö data, that it is primarily the permeability of the rock nearest the tunnel, which is furthermore affected by various grouting measures, that will determine the inflow, although the boundary condition at the surface is also of importance. To be able to judge the resaturation time, groundwater recharge will probably have to be described fairly realistically.

By and large, the input data requirements for the inflow-resaturation calculations probably coincide with the input data requirement for regional groundwater flux and the input data needed for migration models. Additional parameters are permeability distribution around the tunnel (which is affected by grouting) and groundwater recharge in the repository area. Parameters for unsaturated flow are probably not needed. A possible need for such data could be analyzed separately before specific requirements on site-specific data are formulated. On a tunnel scale, additional data are needed that can really only be determined during detailed characterization and repository construction (excavation-disturbed zone, detailed structures, etc.).

5.2.3 Input data to migration models

When groundwater models are to be used as input data to migration models, it is necessary to take into account the fact that the hydraulic properties of the rock vary greatly in space. This results in the formation of different flow paths for the groundwater with differing transport properties.

The flow paths need to be described on a sufficiently detailed scale. It may also be necessary to take into account correlations between flow and other transport parameters (see Chap. 7). As is evident from the discussion in Chapter 7, there is no special study of how detailed a resolution of the flow field is needed, but a reasonable level of ambition ought to be the scale of single deposition holes. On this scale it is not meaningful to describe heterogeneity deterministically – a stochastic description is needed, and different models have been developed for this purpose.

SKB uses (see SR 95) mainly the stochastic continuum model HYDRASTAR to describe detailed groundwater flow, but also has access to discrete network models (FRACMAN) and channel network models (CHAN3D). These models have some overlapping input data needs, although the nomenclature may vary. Other input data needs are more tailored to the individual model and represent different approaches for utilizing information indirectly to describe the flow paths. Site-specific parameters for describing the detailed groundwater flow can thereby not be directly described in terms of the parameters of an individual model. Data need to be independent of the model used and should at the same time be able to be utilized with different approaches.

5.2.4 Source term calculations

Groundwater flow on the near-field scale is included as input data in source term codes. Data needs for these are further commented on in Chapter 7.

5.2.5 Input data to biosphere models

Hydrogeological data, above all from the soil layers, are utilized as input data in biosphere modelling. Quantitative modelling of biosphere transport is done in compartment models such as BIOPATH (see SR 95, 11.5). These models calculate the migration of radionuclides along different transport pathways up to human exposure. For given premises, the results of these calculations can as a rule be presented in the form of equivalent dose factors (Sv/Bq) which are multiplied by the release from the geosphere (in the form of Bq/y) to give the resulting dose rate (Sv/y). In safety assessments performed to date, generic data estimated from assumptions concerning plausible exposure pathways in the biosphere have been used almost exclusively for these calculations. The reason for this has been the large changes that occur in the biosphere within relatively short periods of time. Research activities in this direction are continuing in international cooperation (BIOMOVS-II, 1996).

According to RD&D-Programme 95, however, site-specific databases and assessments of the limits within which the biosphere on a given repository site can change are judged to offer a basis for a relatively meaningful forecast, especially for the next 1000 years. Such modelling is needed if it is to be possible to make comparisons between repository sites and study radiation protection optimization (for example, compare doses arising from operation of the final repository with doses that can otherwise occur in the future). The time horizon of 1000 years for comparisons of this kind is mentioned in a proposal for regulations from the National Radiation Protection Institute, SSI (SSI, 1995).

The input data requirement for biosphere modelling is commented on in general terms in SR 95. Where, when and in what chemical form the release comes from the geosphere are input data from transport modelling of the geosphere (see Chap. 7). Dose factors for external exposure and intake, which must not be confused with the dose factors mentioned above, are dependent on biological factors and radiation protection factors that cannot be site-specific. The site-specific input data requirement for biosphere models therefore comprises to a very large extent hydrological and hydrogeological parameters for the upper soil layers. In general terms, biosphere modelling hereby needs information on receptors (receiving streams, lakes, groundwater reservoirs, deep wells), water flux in and around them and information on changes. The input data requirement for such models is therefore commented on in this chapter, even though strictly speaking biosphere modelling has to do with transport and therefore ought to be discussed in Chap. 7.

Data on the following are required for site-specific biosphere modelling (see English version of SR 95, pp. 102–105):

- *present-day extent of receptors* e.g. conditions for wells, watercourses, lakes, seas, bottom sediments,

- *water flux in receptor* e.g. well withdrawal rate, dilution, and contact with deep groundwaters, water flux and retardation in respective receptor, biological cycling and accumulation,

- *estimates of changes of receptors* e.g. changes in precipitation, water level, silting-up etc.

Retardation in various receptor compartments, which in general is dependent on chemical (sorption) and biological processes, also needs to be described. This is done as a rule using distribution coefficients. The need for site-specific information on this is discussed in Chap. 7.

Essential input data for biosphere modelling also include assumptions concerning the critical group (i.e. those for whom the dose consequences are to be calculated), exposure pathways (e.g. dietary and living habits for the critical group) and data on dose factors for external exposure and intake. To shed light on environmental protection, it may be necessary to extend the analysis to other species than man. Identification of present-day flora and fauna may, for example, be necessary. Collection of this type of input data is probably beyond the scope of the strictly geoscientific site investigation programme, however.

5.2.6 Other near-surface environmental consequences

Besides biosphere modelling as described above, it is highly likely that an environmental impact assessment needs to describe how the deep repository otherwise affects the environment. The level of ambition needed in such modelling work has not be established. The necessary measurements are probably site-specific and can only be partially determined on the basis of feasibility studies and consultations of various kinds. A reasonable ambition should, however, be to perform a traditional hydrological and hydrogeological description of the upper soil layers.

The groundwater flux in near-surface aquifers is relatively independent of the groundwater flux at depth. Conditions on the surface may also change with time. The input data that are needed correspond to the input data needed for a more traditional hydrogeological characterization. For evaluation of near-surface environmental consequences (Land and Environment), traditional (porous medium) models can be used. This modelling can be done independently of the modelling of the hydrogeology in the deep-lying rock.

The input data requirement for this type of modelling is probably identical to a large extent to the input data requirement for biosphere modelling.

5.2.7 Favourable, unfavourable and discriminating factors

In the supplement to RD&D-Programme 92, a number of favourable, unfavourable and discriminating factors are mentioned with a bearing on hydrogeology.

Factors rated as *favourable* were low groundwater discharge at repository level and long flow paths to the biosphere. Factors rated as *unfavourable* were many closely-spaced water-bearing fracture zones with rapid transport pathways up to the surface and highly heterogeneous and difficult-to-interpret bedrock. Factors rated as *discriminating* in the sense that they can occasion abandonment of a site where site investigation has begun were: pronounced groundwater discharge areas and many closely-spaced water-bearing fracture zones.

The selection of factors needs to be discussed, and the factors need to be quantified to be useful. For example, it is highly debatable whether a discharge area should have to be discriminating (except in very special cases), since this would in principle rule out all near-coast areas.

It can in any case be concluded that the above factors can be quantified with the hydrogeological parameters identified in coming sections. In other words, a further definition and possible revaluation of site selection factors can be based on the list of parameters in Appendix A:4.

5.3 Hydraulic properties of modelled discontinuities

Groundwater flow takes place in fractures in the rock. Since the conductivity of a discontinuity is affected by a whole series of factors, there is no obvious correlation between hydraulic properties and the size of the discontinuities. It is, however, reasonable (and is done in practical modelling) to describe deterministically hydraulically significant discontinuities above a given size level. But it should be observed that even if the position of a discontinuity has been fixed deterministically, its properties can still vary in the "plane" of the discontinuity, be uncertain or needed to be described stochastically.

5.3.1 Discontinuities

Description and classification of discontinuities has already been discussed in the section on geology (Chapter 2). Such structure-geological information is valuable in a hydraulic model, provided that identified discontinuities have hydraulic properties that significantly deviate from those of the rest of the rock mass. Major structures are placed directly in flow models, but in view of the limited correlation between measurable discontinuities and flow data, and in view of the difficulty of finding all minor discontinuities, there is hardly any justification (based on data from site investigation) to explicitly incorporate discontinuities below a given scale. Below this scale, however, the varying properties of the rock need to be handled in some way, either as an average or stochastically.

Evaluation of importance, requirements on resolution and measurement methods

Since discontinuities can be important flow paths, information on their geometry is of direct and essential importance for judging the isolating capacity of the rock and for being able to develop a plausible hydrogeological model both on a site scale and for migration models. In a similar manner, the discontinuities are essential for a geoscientific understanding of the site. The geometry of the discontinuities is also essential for layout, construction analysis and working environment (industrial safety). In order to determine whether the discontinuities are also really essential, their hydraulic properties have to be determined. This is discussed in section 5.3.2.

Evaluation of the importance of discontinuities for hydrogeological applications has already been discussed in the chapter "Geology" (section 2.7) and is shown in Appendix A:1. In summary, the following levels of ambition are conceivable:

- identify all hydraulically significant regional discontinuities;
- attempt to identify all hydraulically significant major local discontinuities but describe uncertainties that permit alternative hypotheses regarding location and properties to be put forth, greater precision is required in the vicinity of the projected repository area;
- collect statistical information on local minor discontinuities and individual fractures (the data need for this is commented on in section 5.4.1), especially in the repository area, and describe directly all discontinuities judged to be important.

In view of the amount of work such a level of ambition would entail, however, there is good reason to further examine how great the need for information here really is. Gustafson and Ström (1995), however, point out the need of knowing how discontinuities are related even outside the projected repository area.

In detailed characterization and repository construction, it may be possible to identify, and hydraulically characterize, considerably smaller structures in the immediate vicinity of tunnels and deposition holes. The choice between deterministic versus stochastic data may then be shifted.

5.3.2 Permeability distribution of discontinuities

In general terms, the distribution of the groundwater flow through the rock (and the distribution of hydraulic head if this can be defined) is determined by the distribution of conductivity and applicable boundary and initial conditions. Conductivity is determined by the properties of the fractures, but the effect of this variation differs depending on the scale on which the problem is regarded.

On a small scale, the properties and connectivity of the fractures vary greatly in space, which can also be seen from all field tests (injection tests on a metre scale) performed by SKB and others in crystalline rock (see e.g. the study area investigations, and Vieno et al., 1992). The properties on a larger scale depend on how high- and low-permeable areas are connected on the small scale. It should, however, be observed that strong, but scale-dependent, spatial variation also occurs within a given discontinuity. To be able to decide on a suitable model for groundwater flow, it is therefore necessary to decide which resolution of the flow field ("scale") is needed for the application in question.

There are different models for describing the spatial variation of bedrock conductivity. Roughly, these models can be divided into ***homogeneous porous medium***, ***stochastic continuum***, ***discrete network*** and ***channel network***, which is illustrated in Figure 5-2. Different sub-variants occur. In the continuum models, conductivity is represented by a permeability distribution (or distribution of hydraulic conductivity), but the crucial factor for the properties of the stochastic continuum model are what autocorrelation structure applies to permeability. In the fracture network and channel models, conductivity is assigned (stochastically, as a permeability distribution, transmissivity or conductance) for the individual fractures or channels, but the crucial factor for hydraulic properties is how these individual fractures or channels are interconnected, i.e. their connectivity. The site-specific data required to determine autocorrelation and connectivity are probably closely related. A likely method for determining these model parameters is by interpretation of possible site investigation results, such as injection tests, interference tests etc., with the model in question. For planning of the site investigation, the ambition must therefore be to carry out relevant tests, not simply to deliver input data to each model. This latter work should instead by regarded as a part of the modelling and interpretation work. Input data requirements for the different models are discussed further in section 5.4.

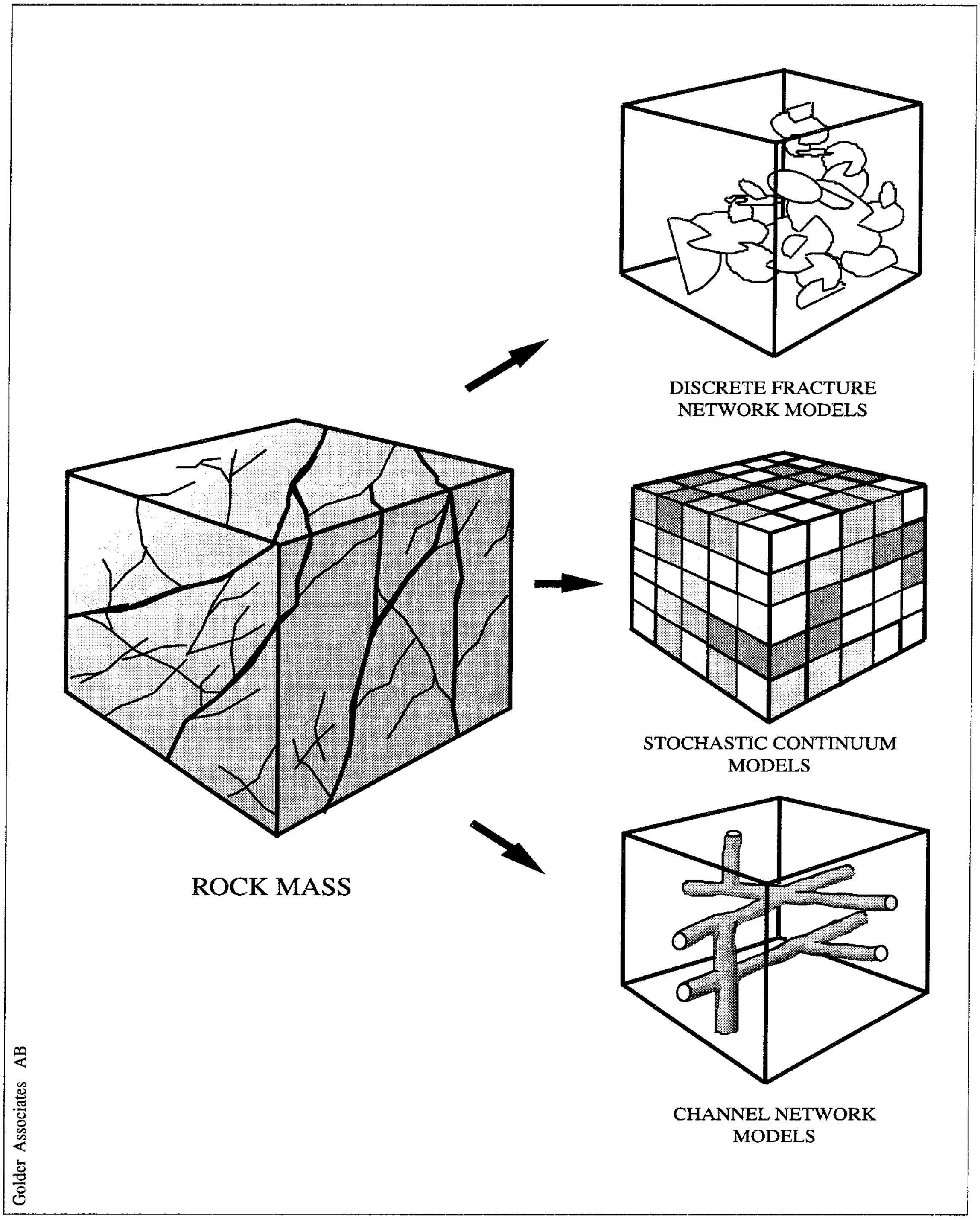


Figure 5-2. Different conceptual models for representing the spatial variation of bedrock conductivity (from Geier et al., 1992a).

The need for resolution is less for hydrogeological modelling on regional and site scales, while the need for resolution is great for models that are to be used as input data to migration models (see section 5.2). There is no established view of whether the variability within the fracture plane can be described as an average or as stochastic variation. For regional modelling an average, with a specified range, is probably satisfactory, but for models that are supposed to deliver input data to migration models higher resolution may be needed. The permeability field within deterministically identified discontinuities situated in the vicinity of the repository area should in the latter case be described stochastically (stochastic continuum, discrete fracture network or channel network).

Since the groundwater can have varying density (and viscosity), conductivity should in principle be described as a permeability distribution over the extent and thickness of the discontinuity. In principle, it is more suitable to use permeability than hydraulic conductivity (which assumes constant density and viscosity) or transmissivity (which is an averaging for two-dimensional structures). There are, however, practical reasons in favour of sometimes using the concepts hydraulic conductivity (i.e. conductivity taking into account the viscosity of the water) and transmissivity (i.e. hydraulic conductivity integrated over a certain length section), see e.g. Bear (1979). The influence of density and viscosity differences on conductivity is relatively limited, and introducing the concept of permeability may be unnecessarily complicated. For discontinuities that are essentially described as homogeneous over their width, it may be more appropriate to talk about transmissivity, which is the parameter that actually controls the flow, and in addition report the zone width in the event conversion to hydraulic conductivity is desired. All of these options are encompassed within the more general concept "permeability distribution" which is given in Table 5-1 and the summarizing table in Appendix A:4.

In practical modelling, the general concepts discussed here must be more precisely defined. Different modelling approaches can (and should) be able to utilize the same basic data, however. That this is possible is demonstrated by how the Äspö Task Force was able to apply different modelling approaches to the LPT2 test (Gustafson and Ström, 1995). This work also shows in practice how the general concepts discussed in this report can be translated into actual model parameters for different models.

Evaluation of importance, resolution and measurement methods

Information on the permeability distribution and connectivity of the discontinuities describes where the groundwater flows in the rock and is thereby of direct and essential importance in a hydrogeological model on a site scale and in migration models. The information is thereby indirectly of essential importance for retention models of the repository area and directly of essential importance for the geoscientific understanding of the site. Similarly, the permeability distribution is of direct and essential importance for the rock's isolating properties as well as for layout, construction analysis and working environment. It should, however, be noted that Windelhed and Alestam (1996) cite the need for transmissivity for discontinuities, i.e. the construction analysis does not have the same need for spatial resolution as models to be used in migration calculations. To some extent, the groundwater flow indirectly influences the integrity of the bentonite and the canister ("erosion" of buffer and supply of corrodants), but the influence is of clearly limited importance. (The evaluation is reported in Appendix A:4.)

Further evaluation may be needed as to what resolution of the information is needed from the following standpoints:

- All regional and major local discontinuities identified in the geological model should in principle be investigated hydraulically to determine whether these discontinuities also need to be included in the hydrogeological model. This requirement can, however, be modified. In a sensitivity analysis, the uncharacterized discontinuities can be assigned different values to examine the need for further precision for different applications.
- The need for resolution of the permeability distribution within the discontinuities is application-dependent. For discontinuities that are close to the projected repository area, i.e. ones that are included in models that are supposed to give flow paths to migration models, the just as high resolution is needed as in the rest of the rock in the repository area (see 5.3.2). The discontinuity here represents only an area with a deviant distribution of properties. For discontinuities located farther away, mean values are probably satisfactory.

Regarding methods for determining the distribution of hydraulic conductivity, see 5.4.2.

5.3.3 "Flow porosity" and "storage coefficient"

In cases where the interior of the discontinuity is described as a porous medium, it is possible to define a porosity for the flowing water within the discontinuity. This flow porosity directly affects the flow velocity for non-sorbing substances and is needed for transient modelling of density flow, input data to transport modelling and for modelling of resaturation (see also section 5.4.3). Flow porosity is also included directly in models for transport of solutes, but is of limited importance for sorbing radionuclides (see Chapter 7). Flow porosity is of essential and direct importance for a geographic understanding of the site, since knowledge of this is needed to be able to judge the rate of changes in groundwater table or transport velocity for e.g. saline waters or other geochemical indicators (see e.g. Voss and Andersson, 1993). The required resolution is however limited.

Porosity is of less importance for determining the groundwater flow rate, even though knowledge of porosity is needed for transient modelling (e.g. interpretation of pumping tests). In the latter case, however, it is more appropriate to try directly to determine the specific storage capacity, which is partially dependent on porosity, but above all on the compressibility of the rock. The storage capacity within discontinuities is of limited importance for the geological understanding, as well as for the construction analysis.

5.4 Hydraulic properties of the rock mass between deterministically modelled discontinuities

Whether discontinuities are treated deterministically or stochastically is partially model- and application-dependent. For models that describe flow paths in migration models, relatively high resolution is needed, and the actual site-specific measurements that are needed are required are roughly the same for both identified structures and the rest of the rock. For regional modelling, the need for resolution is less and here the location of the identified discontinuities can be essential for the positioning of boreholes and measuring equipment in it.

Different modelling approaches, see 5.3.2 and Figure 5-3 above, can be used to describe the groundwater flow in the rock between deterministic discontinuities, but both experience from the Äspö Task Force (Gustafson and Ström, 1995) and SKI's (the Swedish Nuclear Power Inspectorate's) SITE-94 show that the results are dependent on the same basic data, regardless of how the model has been formulated.

5.4.1 Statistical description of discontinuities

Statistical information on minor local discontinuities and individual fractures can be used to describe the permeability distribution in the portion of the rock that is not described with deterministic discontinuities. Different modelling approaches are used, which has already been discussed in section 5.3.2.

Discrete network models use the statistical information directly (see e.g. Geier and Dershowitz, 1992), but the information can also be utilized indirectly in stochastic continuum models (see Winberg, 1994) and channel network models (Gylling et al., 1994ab). Fracture information can, for example, be used to justify an anisotropic correlation structure in indicator simulation with stochastic continuum models (see e.g. SKI, 1996 and Tsang et al., 1996).

Evaluation, need for resolution and measurement methods

The smaller scale determines the detailed distribution of groundwater flow paths. Knowledge of this distribution is needed on a scale corresponding to individual deposition holes if the modelling result is to be utilized in migration models. The stochastic description of smaller-scale discontinuities is thereby directly of essential importance for being able to set up hydrogeological models on a repository scale and thereby indirectly of essential importance for retention models of the repository area. (The evaluation is shown in the table in Appendix A:4.)

Discrete network models can use data on fracture length, fracture frequency and orientation that have been estimated from slices in the rock. The estimates are burdened by uncertainties and are dependent on the assumed geometric model in the discrete model (see further Chapter 2).

It must be remembered that the correlation between observable fracture statistics and hydraulic and transport properties is limited. Compared with direct evidence of the distribution of hydraulic flow paths, the geometric fracture information is of limited value. It is also worth pointing out that information on fracture properties such as fracture filling, aperture etc. is not used in the modelling at the present time. As a rule, the hydraulic properties of the fractures are estimated directly from the hydraulic information.

Stochastic continuum models and channel network models do not need to use the geometric information at all but can theoretically build up their internal geometric structure solely with the guidance of hydraulic data. Gylling et al. (1994a), for example, utilized the permeability distribution in boreholes to estimate channel density and flow-wetted surfaces.

Fracture width and fracture frequency are needed (sometimes) for near-field modelling (see Chap. 7). Information on this can be obtained from the above models, but the predictions need to be checked against direct measurements.

5.4.2 Permeability distribution

The rock mass between modelled discontinuities can still contain significant flow paths, which lead to spatial variation of the flow. The spatial variation is not an uncertainty, but it creates uncertainty, partly regarding what the conductivity is in a non-investigated area, and above all regarding how areas with high conductivity are interconnected.

There are different approaches to describing the conductivity in the rock mass: as a porous medium, as a stochastic continuum, as a discrete fracture network, or as a channel network (see 5.3.2). It is therefore important to ensure that site-specific information is gathered that permits interpretation by means of these different model concepts, while specific parameter values are determined for the individual models as a part of the hydrogeological evaluation. Regardless of model, however, information on the point variation and correlation structure of the conductivity is needed even though the requirements on resolution vary with the intended use of the model.

For models that are supposed to describe the regional groundwater flow, it is probably possible to average measured “point conductivities”. Although the correlation structure influences how this averaging should be done, the results can be checked by means of large-scale pumping tests.

For detailed flow models (to be used for migration and near-field modelling), on the other hand, the correlation structure of the conductivity can be crucial. At greater distances, the properties of the rock are completely different depending on whether local areas of high conductivity are interconnected or are isolated from each other. This applies regardless of the chosen model concept. Which correlation structure has been assumed is of crucial importance for the properties of the stochastic continuum model, and in a similar manner the properties of the fracture network model are determined by the connectivity of high-conductive fractures (see e.g. SKI, 1996).

Evaluation, measurement methods and need for resolution

Permeability distribution and connectivity are directly of essential importance for being able to set up hydrogeological models on a repository scale and thereby indirectly of essential importance for retention models of the repository area (see Appendix A:4). Moreover, the permeability distribution directly influences the groundwater flow in the near field. According to the source term models used today (see section 5.2 above), the local groundwater flow has only a limited influence on the release. The permeability distribution is of direct and essential importance for layout, construction analysis and working environment.

The requirement on resolution of conductivity is relatively limited for the regional modelling. Information from a number of boreholes, combined with large-scale pumping tests, is probably sufficient.

The requirement on precision in information on the variation and correlation structure of conductivity is greatest for models that are supposed to supply data to migration and near-field calculations. In principle, a resolution on a scale in the order of 10 m is needed here (see above). On the other hand, the description can only be made stochastically on this scale.

It is conceivable that a suitable approach is to thoroughly characterize a smaller volume in the repository area and then use this information to extrapolate stochastically to properties in the non-investigated portions of the rock mass. This detailed information should then be augmented with more scattered measurements in the entire rock mass to provide a check of the correctness of the extrapolations and to permit conditioning. However, in view of ongoing research and development work, especially within the Äspö project, it appears urgent that targeted studies be conducted to further explore this question.

The spatial point variation of hydraulic conductivity can be measured by means of injection tests in borehole sections. Transient analysis of such data provides some information on the correlation structure (e.g. estimates of flow dimension), but only of a limited scope and quite inadequate for the needs of migration modelling.

What is really needed are direct measurements of how/if the high-conductive areas of the rock are interconnected ("connectivity"), as has been observed in SKI's SITE-94 and by Gustafson and Ström (1995), among others. This is more important than the choice between stochastic continuum description and discrete networks. Such information could possibly be obtained from cross-hole tests or large-scale tracer tests. Proposals to measure between sections in the same borehole appear interesting, especially if this would enable more cross-hole measurements to be performed (due to the lower cost). The measurement scale (tens of metres) is interesting and relevant.

Flow logging (e.g. with a spinner or TVO/Posiva's differential flow log) provides information on the distribution of points of inflow along a pumped borehole. This and other information on "hydraulic fracture frequency" can, combined with discrete network modelling, provide indirect information on connectivity.

The possibility of alternative interpretations is, however, relatively great and the measurement methods have limited resolution (Rhén ed., 1995).

In conjunction with tunnel construction and excavation of deposition holes, the conductivity of the rock will be altered locally, particularly as a consequence of damages caused by the rock works and to some extent due to changes in the stress situation due to the withdrawal of rock. Degassing and air ingress from tunnels can also disturb the groundwater flow locally. Research on these questions is being conducted within the ZEDEX project (Olsson et al., 1996). The changes will also continue when canisters are deposited, above all due to the bentonite's swelling pressure, the heat load and future climate changes (e.g. ice load). The need for parameters to assess the impact of these changes has already been touched upon in the chapter on rock mechanics (Chap. 3). Preliminarily, generic data can be used during the site evaluation phase to make plausible assessments of these effects.

5.4.3 Flow porosity, storage coefficient, compressibility

Flow porosity influences the flow velocity of non-sorbing substances. Flow porosity is needed for transient modelling of density flow, input data to transport modelling and for modelling of resaturation. Knowledge of this is therefore of essential importance for the geoscientific understanding of a site. To interpret tracer tests, relatively high precision is required in the porosity values, but the question can be asked whether porosity data independent of the tracer test are available (see also Chap. 7). Porosity can be estimated from drill cores, but in the evaluation of tracer tests porosity is generally used as a calibration parameter (see e.g. Gustafson and Ström, 1995).

For direct applications in the safety assessment, the porosity of the rock mass is of subordinate importance. A few measurements, or even generic data, are probably sufficient.

Storage coefficients are needed for transient evaluation of pumping tests, but are of no importance for long-term properties. Gustafson and Ström (1995) believe, however, that independent measurements of storage coefficients would have been valuable to better be able to interpret the tracer test in LPT2. In other words, storage coefficients are of importance for a geoscientific understanding.

The storage coefficient is estimated in connection with a pumping test, but independent data would be valuable (then the pumping tests can be used to estimate other data). An underestimation of the storage coefficient is obtained from the compressibility of the water and the flow porosity of the rock, but in practice the storage coefficient is largely determined by the compressibility of the rock. Geier and Dershowitz (1992) describe how the storage coefficient can be represented in discrete network modelling.

The above evaluation is shown in Appendix A:4.

5.5 Salinity and temperature

The groundwater salinity and temperature influence density and viscosity, and the density and the viscosity influence the electrical conductivity. At reasonably high permeabilities the relationship is linear (see e.g. Bear, 1979). If temperature and salinity are known, density and viscosity can be determined with the aid of literature data.

Density variations due to the thermal evolution of the repository are relatively small. If the natural hydraulic gradient is large, the thermally induced driving force can be neglected (Thunvik and Braester, 1980), but it may have to be taken into account when other driving forces for groundwater flow are lacking. The specifically thermal parameters that are needed to describe temperature-dependent groundwater flow are discussed in Chapter 4.

Of greater interest is the fact that density differences due to salinity influence groundwater flow via lift forces. For the large-scale flow modelling, relatively high precision is needed in determination of the salinity distribution and consequential density differences. Gustafson and Ström (1995) noted, for example, that large uncertainties regarding the distribution of salt water at Äspö in turn led to uncertainties regarding the regional groundwater flow pattern, but that these uncertainties were of little importance in analysis of pumping tests. In modelling of density effects, it is furthermore as a rule necessary to take large-scale changes in boundary conditions into consideration, and vice-versa (see Andersson and Voss, 1993).

The influence by temperature is different between different parts of Sweden. Formally, a measured temperature distribution should be regarded as an initial condition, since heat from the repository will influence the temperature. The temperature due to the repository can be figured out and does not, as a rule, affect groundwater flow significantly. In other words, there is hardly any reason to measure temperature for groundwater flow alone. (See also Chapter 4.)

The above evaluation is shown in the table in Appendix A:4.

Measurement methods

Salinity should preferably be measured for undisturbed conditions (water samples taken during drilling). However, performing such measurements is no trivial matter.

5.6 Hydrogeological data for the soil layers

The hydrogeological data for the soil layers is used primarily for needs in biosphere modelling and other evaluations of the near-surface environment (see

5.2.5 and 5.2.6). To estimate the receptor information and otherwise be able to describe the near-surface environment, the following site-specific hydrological and hydrogeological information is needed (some of this ought to be known already from the feasibility studies):

- *Identification of present-day receptors* (see above). This information is naturally of essential importance for both the biosphere modelling and other analysis of the environmental impact of the repository. The mapping should also include description of ecosystem, biological substrate and vegetation.
- *Meteorological and hydrological data:* To be able to estimate groundwater recharge and water flux in receptors, information is required on precipitation, temperature, air pressure, surface runoff, flows, sea water levels, lake water levels, evapotranspiration etc., but also on various human activities such as dredging, drainage schemes, damming schemes, logging activities, groundwater withdrawal in wells and water supply. The information is of essential importance for site-specific biosphere modelling (even though the requirement on precision is limited in view of the long-range uncertainties), of essential importance for description of land and environment, and of limited importance for the groundwater flow in the rock because it affects the estimation of groundwater recharge. The information can be gathered by customary hydrogeological mapping.
- *Hydraulic conductivity, storage coefficient, thickness etc.* To be able to estimate the groundwater flux in the soil layers and between soil layers and watercourses, traditional data for groundwater modelling is needed such as hydraulic conductivity and thickness of soil layers, storage coefficients and hydraulic conductivity of bottom sediments. This information is of importance for site-specific biosphere modelling and is of essential importance for being able to describe other environmental impact in the biosphere. The requirement on precision varies. The information can be obtained from soil type composition (see geology) combined with pumping tests.

For biosphere modelling it is also essential to be able to estimate dilution in the geosphere and in the interface between geosphere and biosphere. Such estimates can, however, be done with the near-surface information described above, combined with groundwater modelling on a site scale. The input data requirement for the latter has already been discussed in previous sections in this chapter.

5.7 Boundary conditions and supporting data

As a rule, hydraulic data cannot be determined directly, but are determined indirectly via e.g. interpretation of pumping tests or extrapolation from assumptions (e.g. position of different structures). There is therefore a need for data that can be used to verify/validate the assumptions made – even though these data cannot be said to measure a given property. Furthermore, boundary conditions are needed for the modelling.

Evaluations of importance for the different parameters discussed below are shown in the table in Appendix A:4.

5.7.1 Regional boundary conditions, historic and future evolution

In large-scale groundwater models, boundary conditions are formulated in the form of specified pressure (head) or specified flow (usually in terms of a zero flow at boundaries assumed to be impermeable). Based on classical theory for groundwater flow it is observed in RD&D-Programme 95 that: "The local topography at a repository area with small height differences probably has very little to do with the flow conditions at the repository level. The flow at the deep repository is then determined by regional gradients." The regional boundary conditions are naturally essential for the modelling results and for a geoscientific understanding of the site.

As a rule, large-scale boundary conditions are estimated indirectly from topographical and geological information. However, the boundary conditions are altered by climate changes which can lead for example to sea level changes, permafrost or glaciation (see e.g. Boulton and Payne, 1993 or King-Clayton et al., 1995).

Today's groundwater situation, with its distribution of saline waters, is moreover the result of an historic evolution. Information on the future evolution of the climate is generic in the sense that it does not directly require data from a site investigation, even though postulated climate changes vary between different sites in Sweden. To relate today's conditions to those in the past, however, site-specific paleohydrogeological information (see e.g. Wikberg et al., 1995) can be important. This is further discussed in the chapter on geochemical parameters (section 6.5).

5.7.2 Pressure and head

Boundary conditions for a hydrogeological model are given in the form of either pressure or flow. Pressure, head and gradients are thereby of essential importance for groundwater flow rate, layout, construction analysis, working environment, as well as geoscientific understanding.

Measurements of pressure and head have two complementary purposes. They can be used to:

- estimate gradients and boundary conditions, whereby mainly pressure under undisturbed conditions is needed,

- calibrate/validate proposed models, whereby it is interesting to relate pressure changes to known disturbances.

Measured pressures are mainly used in large-scale rock models. The topographical information provides good opportunities to estimate the gradient, but a direct check that the assumptions made are reasonable is valuable and necessary.

Pressure determinations and setting of boundary conditions are complicated by density variations. The driving force is then determined by the combination of pressure gradient and density gradient. The salinity of the deep waters at Äspö, Laxemar or other near-coast sites is definitely of such a magnitude that it has to be taken into account. A further complication, which is directly connected to this, is that the large-scale systems are not in equilibrium. The highly saline water can be in movement to compensate for near-surface pressure changes resulting from postglacial land uplift and other sea level changes (Voss and Andersson, 1993).

Pressure measurements are also complicated by the fact that the pressure is sensitive to disturbances. If new boreholes are drilled or packered boreholes are opened, this may result in large pressure changes. This can in itself be an advantage, if the disturbance is known and can be quantified, but entails difficulties in practice.

Even though different models can be calibrated against pressure data, which has for example been demonstrated by the Äspö Task Force (Gustafson and Ström, 1995), such a calibration allows wide possibilities for interpretation of the more detailed permeability distribution. The potential for utilizing pressure data for determining connectivity is very limited. The gradient is determined above all by regional conditions and is roughly the same over homogeneous and heterogeneous sections of the rock. In other words, measured pressures (in MPa) and densities can be used for verification of modelling results, but cannot be inserted directly into model calculations.

Groundwater pressure varies over time because it is influenced by air pressure and tidal forces. The tidal forces cause a periodic fluctuation where the driving force (gravitation) is known, but the resulting pressures are affected by the structure and compressibility of the rock. It has been discussed whether this information could be used to obtain information on the hydraulic (and mechanical) properties of the rock mass. There are no practical methods available for this today, however. Such methods therefore need to be developed if they are to be used in a site characterization programme.

Roughly the same principles apply for near-surface groundwater models as for large-scale models as described above. The potential for utilizing pressure data for calibration is, however, greater than in the rock, since a larger number of measurement points can be obtained at a reasonable cost.

Measurement methods

Groundwater pressure can be measured in packer-sealed boreholes. In view of the long-term fluctuations of the pressure, it should be monitored over extended periods. Measurement values from a single occasion cannot be used reliably. The measurement should preferably measure pressure (MPa) and not head or groundwater table. These latter quantities can be calculated for known density variations. The influence of air pressure and tidal forces needs to be compensated for. There is a risk that short measurement sections will not be representative, whereas long measurement sections can entail short-circuiting effects.

The large-scale change in boundary conditions is information of a generic type, even though it varies between different sites (latitude, near-coast or inland). Information on the large-scale salinity distribution is also probably obtained mainly from already available data (e.g. the well archive). It needs to be supplemented with more local measurements, however.

Pressure boundary conditions for small-scale models are mainly obtained as modelling results from the large-scale models.

No targeted study has been carried out to investigate what a proper spacing between measurement points should be, particularly if the density of the groundwater varies. Simulation exercises with Äspö data and groundwater models developed for Äspö could be carried out for this purpose. In view of how measured pressures are used today to provide boundary conditions (or as supporting data, see below), there is no reason to drill more boreholes for pressure measurements than those drilled for other hydraulic tests. For a regional modelling, however, it is valuable to have information from boreholes outside the repository scale. Information from the Laxemar holes has, for example, proved valuable for understanding conditions at Äspö. If such "regional" boreholes are to be meaningful, however, they need to be drilled to great depths, greater than in the repository area itself, since the depth of the regional groundwater flow that could conceivably affect the repository area increases with the distance from the repository area.

5.7.3 Recharge and discharge areas

Characterization of recharge and discharge areas provides important boundary conditions for groundwater models. The information is generally utilized indirectly, i.e. boundary conditions and assigned model properties should result in a flow model that recreates recharge and discharge areas. In the case of rock models, however, near-surface areas do not have to be directly correlated to flow conditions at depth – the uncertainties are great. For example, Gustafson and Ström (1995) conclude regarding the LPT2 tests at Äspö that the infiltration rate that reasonably applies for the deep groundwater there (about 5 mm/y) can deviate widely from annual precipitation and superficial groundwater recharge (about 150 mm/y).

If it can really be established that a given area is a discharge or recharge area for deep-flowing groundwater, this is naturally useful information. It should be used to calibrate the groundwater model so that it does not yield results in conflict with these data. If, for example, flow path calculations show that leakage from the repository flows out into a certain fracture zone, it would be interesting to make measurements of the geochemical signature of the water in the fracture zone that show that it discharges deep groundwater.

The possibility of groundwater recharge is interesting for groundwater modelling during the construction and operation phases.

Near-surface models (Land and Environment) have a more direct use of recharge and discharge areas for boundary condition formulation.

In a longer time perspective, it is important to taken into account the large-scale changes in groundwater recharge that occur due to e.g. permafrost, sea level changes or glaciation. It is hardly realistic to expect any great precision (in surface distribution) in these changes. Modelling of the consequences of such large-scale changes is mainly done in the large-scale models.

Measurement methods etc.

Further study may be necessary regarding which data are really needed and what level of ambition is reasonable. But it appears to be a reasonable point of departure that the near-surface data that are collected for the near-surface hydrogeological description needed for Land and Environment are more than sufficient to assess the influence of projected final repository depth.

5.7.4 Large-scale tracer tests

Large-scale tracer tests can provide valuable complementary information to the purely hydraulic data. If a tracer has been transported between two points, this is incontrovertible proof of contact. However, the possibilities of alternative interpretations and other uncertainties with tracer tests prevents the information from being used directly for parameter estimates. Large-scale tracer tests can, if breakthrough has really been established, provide essential, albeit indirect, information on the reliability of groundwater models on a site scale.

5.7.5 Groundwater flow in boreholes

If it were technically possible it would be very valuable to get direct measurements of the groundwater flow in the rock. This information could be used to calibrate flow models, but could also be used directly in near-field and migration models.

At the present time, however, it appears as if flow measurements (dilution probe) cannot be used for this purpose. Rhén ed. (1995) concludes, for example, that flow measurements in conjunction with interference tests, as well as flow measurements under undisturbed conditions, can be interesting, but advantages and disadvantages should be analyzed. Theoretical problems include skin effects, scale and resolution.

Measured groundwater flows can therefore as a rule only be used to check if predictions of flows made with models are plausible. Above all, it should be appreciated that predictions of flows on the scale on which the measurements are made can only be made stochastically. Exact agreement between measured and calculated flows is presumably not a reasonable level of ambition; on the other hand, it can be interesting to recreate the distribution of measured flows. Good flow data and a groundwater model that recreates the distribution of these data ought to be a strong argument for the plausibility of connectivity assumptions. In view of the theoretical advantages, the utilization of flow measurements should be further examined.

6 Chemistry

6.1 Overview of parameters, measurement methods and areas of application

Table 6-1 summarizes, very briefly, what chemical information is needed to build up a geoscientific understanding of a site and to furnish the information that is needed in performance and safety assessments. The parameters in Table 6-1 are found, in more detailed form, in the collected parameter table in Appendix A:5. The recommendations offered in this chapter are based on experience gained from the Stripa Project (Andrews et al., 1988) and from the pre-investigation phase of the Äspö Project (Smellie and Laaksoharju, 1992), and on general experience from Sweden and Finland (Laaksoharju et al., 1993).

Table 6-1. Overview of data requirements for geochemical description, measurement methods and areas of application.

Parameter	Method	Used for
Groundwater chemistry in the repository area Various chemical parameters – specified below	Analysis of groundwater sample Evaluation	Geochemical model. Canister performance, bentonite performance, fuel dissolution.
Groundwater chemistry along flow paths Various chemical parameters – specified below	Analysis of groundwater sample Evaluation	Geochemical model. Rule out transport mechanisms.
Groundwater chemistry on site scale Various chemical parameters – specified below	Analysis of groundwater sample Evaluation	Geochemical model/understanding Prediction of long-term changes.
Mineralogy Various minerals – see below	See geology (section 3)	Geochemical model/understanding.

6.2 Models and areas of application

A groundwater chemistry model comprises an important tool for many analyses. The model is largely based on collected water samples, but also needs information from geology and hydrogeology. This is illustrated in Figure 6-1.

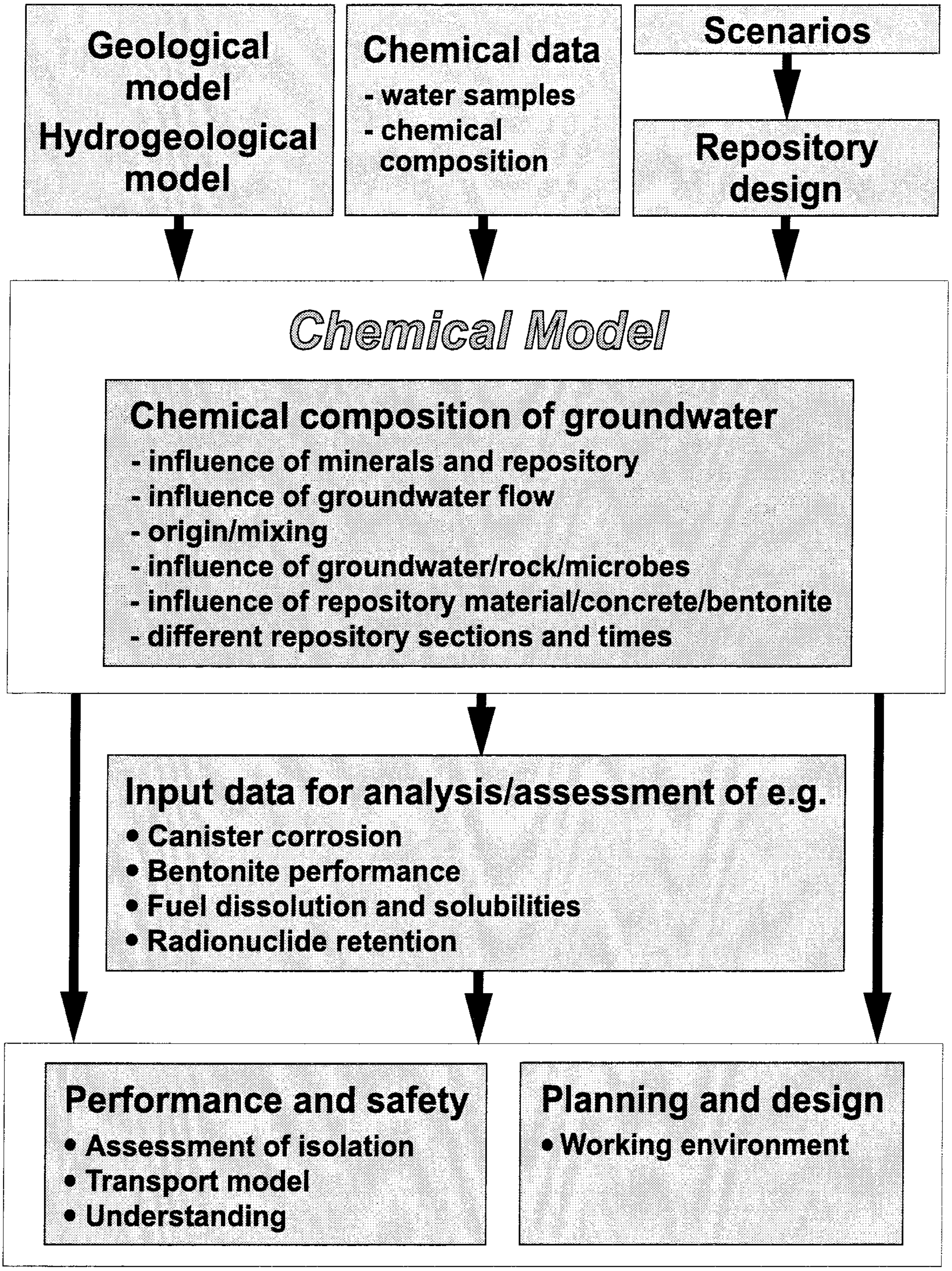


Figure 6-1. Schematic illustration of structure and use of a groundwater chemistry model.

6.2.1 Assessment of repository performance

The description of the groundwater chemistry on the site and at the depth being considered for the repository is an important part of a safety assessment. Normally the information is presented in the form of a table, which can also contain possible variations in composition. The water composition is used later to evaluate different processes of importance for safety or as direct input data for calculations, e.g. to the calculations of solubility and speciation of radionuclides that are usually included in a safety assessment for high-level waste. In summary, the groundwater chemistry is of importance for assessment of:

- canister corrosion,
- bentonite performance,
- fuel dissolution and solubilities,
- radionuclide retention,
- geoscientific understanding.

Calculations of radionuclide solubility are done with thermodynamic equilibrium programs, such as EQ3/6 or PHREEQE, as described in SR 95, 10.6. These programs calculate solubilities at equilibrium and speciation for a given system.

The importance of different hydrochemical parameters for the safety assessment can vary quite a bit and is highly dependent on which scenario is considered likely, and naturally the development of other knowledge in the field. If, for example, it can be shown with certainty that the canister is always intact and remains intact, the influence of water on radionuclide chemistry loses all importance. If, on the other hand, one is extremely pessimistic regarding the capacity of the canisters to isolate the waste and assumes that they fail early on, long before they corrode, then it is of no importance whatsoever whether the water contains anything that might cause corrosion. This is a purely hypothetical extreme example, but the fact is that safety assessments performed at different times have differed quite a bit in some of their assumptions. This underscores the fact that one cannot focus too narrowly on the analysis needs that exist today. It must be remembered that one and the same site will be subjected to many safety assessments, and it is wise to exercise a little foresight regarding water chemistry the day a safety assessment is performed with the intention of closing the facility after perhaps 40–50 years of operation. Not only may the needs change during this time, it will also be difficult to perform supplementary measurements in a facility that has been open so long.

6.2.2 Groundwater chemistry model

The water composition that is used to make the above assessments does not have to be completely identical to the groundwater chemistry that has been measured. A geochemical model (Figure 6-2) that in principle is capable of describing the chemical composition of the groundwater in different parts of the rock and how this chemistry will change needs to be set up (see e.g. SR 95, section 6.3).

Uncertainties in measured data need to be handled. It may be necessary to select conservative values from water samples of differing composition. Furthermore, the

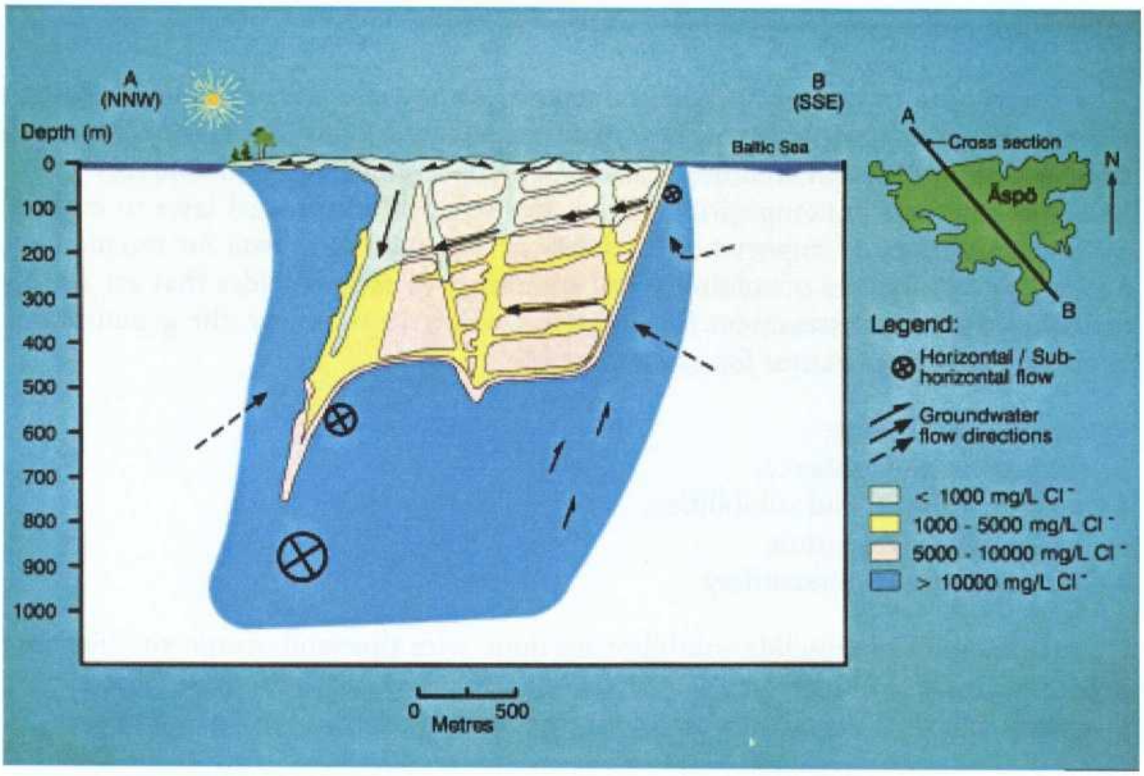


Figure 6-2. Groundwater chemistry model for Äspö (from SKB SR 95).

composition of the groundwater may change on the near-field scale when it comes into contact with the bentonite, the canister, corrosion products and the spent fuel.

In the long term, large-scale groundwater movements could also influence the groundwater chemistry on a repository scale due to the fact that groundwater of another chemical composition is transported there. A key to being able to predict the future evolution of groundwater composition is thereby an understanding of the origin (genesis) of the groundwater. Examples of processes that need to be evaluated are the post-closure recovery of water table drawdown and the impact of glaciation. Analyses can be performed qualitatively and can be supplemented by regional hydrogeological analysis with time-dependent boundary conditions.

A geochemical model is based on a combination of quantitative calculations and qualitative assessments. In SR 95 and in earlier safety assessments, the results of the geochemical modelling are presented in the form of a reference water with uncertainties. For scenarios that deviate greatly from the "normal case", alternative water compositions can be formulated.

6.2.3 Favourable, unfavourable and discriminating factors

In the supplement to RD&D-Programme 92, a number of favourable, unfavourable and discriminating factors are mentioned with a bearing on water chemistry.

Factors rated as *favourable* were: pH 6–9, reducing conditions, plausible salinities, plausible concentrations of humic and fulvic acids, i.e. "normal conditions in deep groundwaters. Factors rated as *unfavourable* were: presence of oxygen, extreme pHs, extremely low or high salinities, high concentrations of humic and fulvic acids, high concentrations of sulphate-reducing bacteria (should really be preconditions for high biological activity of such bacteria), high concentration of total organic carbon (TOC), and high concentrations of nitrogen compounds. A factor rated as *discriminating* in the sense that it can occasion abandonment of a site where site investigation has begun was extreme groundwater chemistry, for example oxidizing groundwater.

The identification of geochemical parameters in the following sections includes all the parameters mentioned above. A further definition of groundwater chemistry site selection factors can, in other words, be based on the list of parameters in Appendix A:5.

The following review shows that it is primarily the presence of oxygen in the groundwater that could be unfavourable for the performance of the final repository, since it directly influences canister corrosion and solubilities of important radionuclides. Normally the boundary between oxidizing and reducing waters is not deeper than 100 m, and in most cases it is much shallower than that. If, on the other hand, the groundwater at planned repository depth should prove to be oxidizing and contain considerable quantities of dissolved oxygen, this should occasion abandonment of the investigated site. None of the groundwater chemistry parameters given above is assumed to have such great direct influence that it could be discriminating by itself

6.3 Groundwater chemistry in the repository area

6.3.1 Groundwater chemistry parameters of importance for the canister

The copper canister is attacked by oxygen or by sulphide. Oxygen can cause so-called "pitting" and is therefore more troublesome than sulphide. Oxygen is normally not present at repository depth, and sites that have high concentrations of oxygen in the water can and should be avoided. The presence of oxygen is indicated sensitively by Eh measurements, whereby normal values of $Eh < 0$ V are a guarantee of the absence of oxygen. Traces of oxygen are enough to influence Eh. The concentrations of Fe^{2+} and HS^- are measured at the same time. They react with oxygen and show by their presence that the water is oxygen-free.

Bentonite also provides some protection against oxygen, partly because it is assumed to react chemically with dissolved oxygen, and because it acts as a transport barrier on the path to the canister. A minimum quantity of oxygen is required for the canister to be penetrated, and water has a limited capacity to dissolve oxygen (Henry's Law). The ability of the bentonite to retard the attack is therefore also an essential protection.

In addition to the bentonite, the rock's content of Fe(II) mineral and sulphides also provides protection against oxygen. To the water's content of reducing dissolved iron(II) and sulphide can also be added the organic compounds that can consume oxygen via bacteria. The latter has proved to be a significant process in conjunction with infiltration of water in the rock (Banwart ed., 1995, The redox experiment, project summary and performance assessment implications). A limited quantity of dissolved organic matter is thus not disadvantageous and can vary between about 1 and 10 mg/l in the groundwater. (The quantity of organic matter in the groundwater is measured as total quantity of organic carbon in solution, Dissolved Organic Carbon, DOC). The concentrations are lower at greater depth.

Sulphide, i.e. HS^-, is itself a corrodant and the concentration is therefore of interest to know. The concentration of sulphide in the groundwater is low in cases where it occurs and is seldom over 1 mg/l. Sulphate can be reduced by bacteria to sulphide with the aid of such reducing agents (electron donors) as dissolved organic matter or the dissolved gases H_2 and methane. Sulphate is often present in the groundwater and the concentration can be relatively high. Furthermore, sulphate is present in the bentonite clay and the bentonite's pore water can have a higher sulphate content than the groundwater. The quantity of sulphate is hardly a corrosion-limiting factor, but the quantity of organic matter or hydrogen gas and methane that must be present as reductants (electron donors) is. Bacteria must take part, and their living conditions are likewise of importance. Mass transport can also constitute an essential limitation. In summary, it is of importance when it comes to sulphide corrosion to be aware of the groundwater's content of sulphide, sulphate, DOC, hydrogen and methane. Furthermore, the repository's own contribution in the form of sulphate from bentonite, organic matter etc. must be estimated, and last but not least the living conditions for sulphate-reducing bacteria must be considered (supply of water, nutrients, etc.).

Deep groundwaters can have a high chloride content. This is not alarming in itself, but extremely high concentrations could increase the sensitivity of the copper canister to pH. It is therefore essential to measure the concentration of chloride in the groundwater and predict future variations in chloride concentration.

High levels of nitrogen compounds such as nitrate, nitrite and ammonium are not desirable since they can cause stress corrosion cracking in copper. Nutrients in general, such as phosphate, nitrate and ammonium, are undesirable since they stimulate the growth of bacteria.

Table 6-2 shows which groundwater chemistry parameters are of importance for the canister. The reasons for the assessment have been given above. The information is also shown in the column Isolation/Canister in the summarizing table in Appendix A:5. (Essential importance = E, Limited importance = L).

Table 6-2. Groundwater chemistry parameters of importance for the canister.

Importance	Parameter
Essential	Eh, Fe^{2+}, HS^-, Cl^-, NO_2^-, NO_3^-, NH_4^+
Limited	pH, SO_4^{2-}, DOC, dissolved gases i.e. H_2 and CH_4, HPO_4^{2-}, HCO_3^-, bacteria

6.3.2 Groundwater chemistry parameters of importance for the bentonite

Excessively low concentration of cations such as Na^+, Ca^{2+} and Mg^{2+} are not so good for the bentonite clay, since they can destabilize the bentonite gel. The gel is then converted to colloidal particles, which can be carried off with the groundwater. Material losses could theoretically be obtained in the buffer in this manner, and besides colloids are never desirable since they can act as carriers of radionuclides. The divalent cations are most important for the stability of the bentonite gel, and the concentration of e.g. calcium ions should preferably be above 0.1 mM (4 mg/l). This is a moderate requirement, which is practically always fulfilled. If the level is clearly below, it should be considered what this entails. The bentonite itself contains quite a few dissolved ions, so it has some ability to protect itself during the time that would be required to leach out the buffer.

Excessively high concentrations of dissolved salts are not desirable either, although the bentonite has a high tolerance in this respect. Water with such high concentrations as to be considered a brine should in any case be avoided.

The clay mineral montmorillonite lends the bentonite clay its valuable swelling properties. Potassium ions can react with montmorillonite, which is thereby converted to illite, whereby the bentonite loses much of its ability to swell. The reaction requires relatively high temperatures, and the mass transport of potassium to the bentonite is also an essential limitation. Nevertheless, it is of course desirable that the concentration of potassium in the groundwater not be extremely high. The concentration of potassium in the groundwater is generally below 20 mg/l.

Diffusion of cesium and strontium in bentonite is important because radionuclides of Cs and Sr are abundant in spent fuel and they are solible and relatively mobile. Cs^+ and Sr^{2+} are sensitive to the salinity of the pore water, since they are bound by ion exchange (chiefly). Diffusivity, which influences retardation in the buffer, is thereby dependent on the ionic strength of the pore water.

Table 6-3 shows which groundwater chemistry parameters are of importance for the bentonite. The reasons for the assessment have been given above. The information is also shown in the column Isolation/Bentonite and in Retardation/ Bentonite in the summarizing table in Appendix A:5.

Table 6-3. Groundwater chemistry parameters of importance for the buffer.

Importance	Parameter
Essential	K^+, Na^+, Ca^{2+}, Mg^{2+}, TDS (Total Dissolved Solids)
Limited	pH, Al^{3+}, SiO_3^{-2}

6.3.3 Groundwater chemistry parameters of importance for fuel dissolution

The dissolution of the fuel is influenced by such groundwater parameters as pH, redox conditions and carbonate concentration. Now the fuel will be surrounded by several tonnes of iron (iron canister) and bentonite, which should play a crucial role for the chemistry in a damaged canister. The iron can control the redox conditions and the bentonite takes on great importance for pH and carbonate concentration. All the same, it is important that the water not contain e.g. oxygen, since it is difficult to demonstrate equilibrium everywhere in a heterogeneous and to some extent dynamic reaction system. Table 6-4 summarizes which groundwater parameters are of importance for the fuel. The reasons for the assessment have been given above. The information is also shown in the column Retardation/Fuel in the summarizing table in Appendix A:5. (Essential importance = V, Limited importance = L).

Table 6-4. Groundwater chemistry parmeters of importance for the fuel.

Importance	Parameter
Essential	Eh, Fe^{2+}, HS^-
Limited	pH, HCO_3^-

6.4 Groundwater chemistry along flow paths – radionuclide retention

The retention properties of the rock are determined primarily by the groundwater flow coupled with matrix diffusion, which permits sorption of solutes on the rock's microfractures. The coupling with the groundwater flow and the importance of clay minerals and porosity conditions are discussed in the next chapter (Chap. 7). The groundwater chemistry along the flow paths is of great importance, since it influences sorption and possible transport mechanisms. Table 6-5 summarizes which groundwater chemistry parameters are of importance for this. The reasons for the assessment are given below. The information is also shown in the column Retardation/Rock/Retention in the summarizing table in Appendix A:5. (Essential importance = V, Limited importance = L).

Sorption that is affected by ion exchange, for example sorption of Sr^{2+} and Cs^{+} on the rock's minerals, is directly dependent on the concentration of other cations in the water. The solubility and mobility of U, Np and Tc are very sensitive to redox conditions. Carbonate forms complexes with, and the pH influences the hydrolysis of, several important actinides, for example Pu and Am. Humic substances can form complexes with radionuclides and in this way change their chemical properties.

Colloidal particles can take up radionuclides and act as carriers. Gas bubbles and bacteria can also act in this manner and are thereby of importance for the migration of radionuclides from a repository. Precipitation of minerals such as calcite and oxides/hydroxides of iron and manganese can bind radionuclides by co-precipitation.

Table 6-5. Groundwater chemistry parameters of importance for radionuclide.

Importance	Parameter
Essential	pH, Eh, Fe^{2+}, HS^{-}, HCO_3^{-}, Cl^{-}, Na^{+}, Ca^{2+}, HA/FA, dissolved gases i.e. N_2, H_2, CO_2, CH_4, He, Ar and colloids and bacteria
Limited	SO_4^{2-}, HPO_4^{2-}, F^{-}, HS^{-}, Fe^{2+}, Mn^{2+}

6.5 Water chemistry for geoscientific understanding

As a rule, groundwaters of differing composition are encountered on one and the same site. The variation in composition, concentrations and chemical properties is greatest with depth, but there are also plenty of examples of horizontal variations. These variations need to be determined for several reasons:

- They explain why the water is like it is at repository depth.
- They indicate possible future variations in composition and properties in both short (e.g. changes due to construction and operation) and long (e.g. ice age) timescales.
- They provide a means of checking hydraulic models for the site.
- They give an indication of the hydraulic transport of solutes (e.g. corrodants and radionuclides) under undisturbed conditions.

In order to get good results, relevant samples taken in several boreholes and at different depths are needed, along with careful evaluation. Multivariate analysis has proved to be a useful tool for revealing mixtures of waters of differing origin/composition.

One should also have a good idea of what minerals are present on the site. This applies particularly to relatively soluble minerals (e.g. anhydrite), those that are reactive in other ways (e.g. clay minerals), and those that could reveal the historical evolution of the area (e.g. iron(III)minerals). Table 6-6 summarizes which groundwater chemistry parameters are of importance. In principle, all of these are also of essential importance, which is also shown in the summarizing table in Appendix A:5 under the heading "Geoscientific understanding".

Table 6-6. Parameters of importance for geochemical understanding.

Parameters
pH, Eh
Main components e.g. Na, K, Ca, Mg, HCO_3, SO_4, Cl
Trace substances e.g. Fe, Mn, U, Th, Ra, Si, Al, Li, Cs, Sr, Ba, HS, I, Br, F, DOC
Dissolved gases e.g. N_2, H_2, CO_2, CH_4, Ar, He
Stable isotopes e.g. ^{18}O & ^{2}H in H_2O, ^{13}C in DIC and DOC, ^{34}S and ^{18}O in SO_4 and HS, $^{87}Sr/^{86}Sr$, ^{3}He, ^{4}He Radioactive isotopes e.g. T, ^{14}C in DIC and DOC, $^{234}U/^{238}U$, ^{36}Cl
Bacteria
Minerals: Soluble, reactive, ones that reveal the evolution of the area

In the compilation of input data requirements for planning and design of the rock works (Windelhed and Alestam, 1996), it is reported that information is needed on pH, electrical conductivity, chemical composition and radon. The requirement on precision regarding pH, electrical conductivity and chemical composition is not explained and should not be so great that it cannot be satisfied by similar requirements made from a geoscientific/safety perspective. On the other hand, concentrations of U and Rn in the groundwater can have a great influence on what ventilation arrangements are needed to maintain an acceptable working environment in the rock chambers. The chloride content of the groundwater can be essential for assessment of the environmental consequences of drainage. The information is presented in the summarizing table in Appendix A:5.

6.6 Quality and requirements on resolution for the groundwater chemistry data

The above discussion shows that the chemical composition of the groundwater comprises necessary information for safety and performance assessments, but also that the same information (e.g. Eh) is important in a number of different contexts. This is also evident from the compilation of the geochemical parameters in Appendix A, which is arranged parameter by parameter.

In view of the varying data needs for different safety assessments in different contexts, as discussed in the introduction, it is not reasonable to limit the chemical sampling in site investigations to those parameters deemed to be most important. All listed parameters should be determined.

The requirements on quality in sampling and analysis of groundwater for the safety assessment are rigorous. This is quite necessary, since the extreme values are generally chosen to test the importance of an unfavourable case. A single incorrect extreme value can easily lead to unnecessarily conservative assumptions in the safety assessment. Furthermore, it is not always possible to repeat samplings of groundwater at a later time after hydrotests or other major invasive procedures have been performed which have altered the original conditions on the site.

To obtain groundwater chemistry data of sufficiently high quality, the groundwater chemistry sampling should therefore be carried out before the hydraulic tests or at least be coordinated with the hydraulic measurement programme.

Regarding requirements on resolution (number of sampling points etc.), this is discussed Laaksoharju et al. (1993) and in Smellie ed. (1993).

7 Retention properties - radionuclide transport

7.1 Overview of parameters, measurement methods and areas of application

Table 7-1 summarizes which data/parameters are needed to describe the retention properties of the rock, i.e. its ability to retard or retain radionuclides dissolved in the groundwater. The table also shows examples of which measurements can be used to estimate the parameters and how they are used. The parameters in Table 7-1 are also found in the collected parameter table in Appendix A:7.

Table 7-1. Overview of data requirements for description of the retention properties of the rock, plus measurement methods and areas of application.

Parameter	Method	Used for
Properties on near-field scale		
Groundwater chemistry	See chemistry data	Parameters in source term model (solubilities, sorption). Assess stability of canister, bentonite (see Chap. 6).
Groundwater flow	From groundwater model	Source term model (Canister corrosion).
Fracture aperture, geometry	Geological mapping, hydrogeological model	Source term model (Canister corrosion).
Properties of flow paths		
Flow paths	Particle track from hydro model	Transport model.
Groundwater flow in flow paths	Particle track from hydro model	Transport model.
Dispersion (long., trans., Pe)	Particle track from hydro model Tracer test	Transport model.
Flow porosity	Tracer test/hydro model	Transport model.
Flow-wetted surface	Lab test, Discrete fracture model, tracer test	Transport model.
Properties of rock along flow paths		
Sorption data (Kd)	Lab test, gw chemistry (in situ)	Transport model.
Matrix diffusivity	Lab test, drill core	Transport model.
Matrix porosity	Lab test, drill core	Transport model.
Max. penetration depth	Lab test, drill core	Transport model.
Density of rock matrix	Lab test, drill core	Transport model.
Groundwater chemistry	Groundwater chemistry model	Determine sorption data.
Transport properties of soil layers/receptors		Biosphere models, land and environment.
Water flux	Hydr. receptor model	
Flow porosity	Soil type mode	
Sorption properties	Soil type model/lab test	
Biological activity		
cont'd. on next page		

Parameter	Method	Used for
Supporting data		
Breakthrough curves	Tracer test	Validation/calibration.
Chemical analysis, fracture filling	Core mapping and analysis	Geoscientific understanding.
Chemical analysis, wall rock	Lab test on drill core	Geoscientific understanding.
Groundwater chemistry, colloids, gas etc. in groundwater	Groundwater chemistry – see Chap. 6	Rule out other transport mechanisms. Geoscientific understanding, predictions of changes.

7.2 Models and areas of application

The transport models that are used in the safety assessment obtain much of their data from the geoscientific description of hydrogeology and geochemistry. The model concepts are often directly adapted to a safety assessment point of view, where actual but difficult-to-characterize mechanisms are simplified in a conservative direction. It can therefore be discussed whether nuclide transport models constitute a part of, or are rather based on, the geoscientific description. On the other hand, transport modelling makes new demands on site-specific data that are not automatically satisfied by the hydrogeological or geochemical description. This is illustrated in Figure 7-1. It is this data requirement that is discussed in the present chapter.

7.2.1 Transport in the near field

The groundwater flow, the retention properties of the rock and the groundwater chemistry in the vicinity of the deposition holes influence – together with the properties of the fuel, the canister and the bentonite – the size of the release in the event a canister has failed. In a similar manner, these properties can also influence the stability of the canister due to the fact that the groundwater can be a source of corrodants.

7.2.2 Transport of radionuclides that have escaped from the repository

The retention properties of the rock are above all of importance in the safety assessment's calculations of transport of radionuclides that have escaped from the repository. Such transport calculations comprise an essential component of a safety assessment. For example, the transport model FARF31 (Norman and Kjellbert, 1990) forms a part of the "calculation chain" illustrated in Figure 7-1, but there are also alternative models. The data needs for these models are, however, similar to each other.

The data needs shown in Table 7-1 largely correspond to the data needed for the safety assessment's migration models, or the data needed, together with other information, to determine such directly necessary data. The modelled transport processes are illustrated in Figure 7-2. It can be noted in this context that the term "rock matrix" which is often used in transport modelling contexts has no

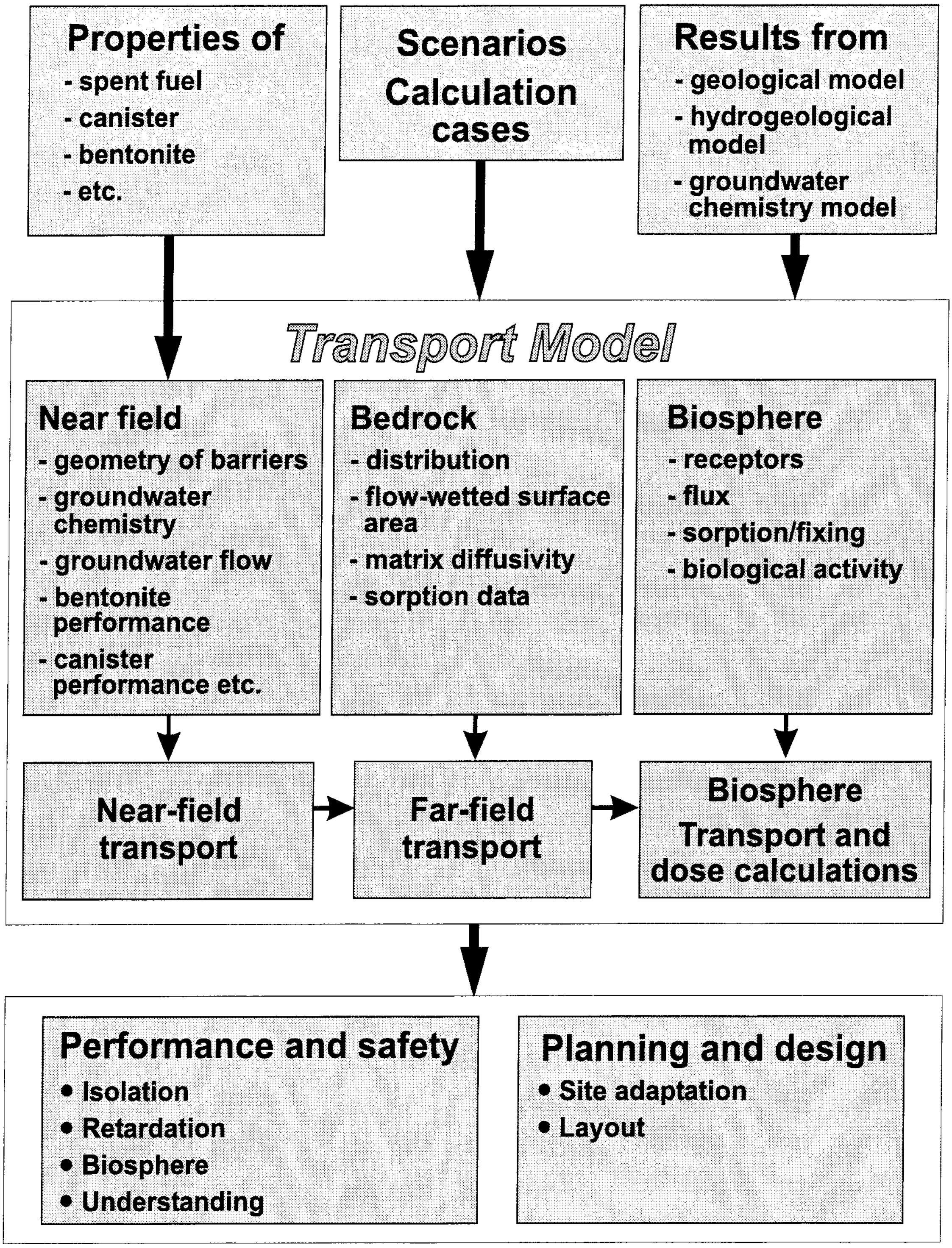


Figure 7-1. Schematic illustration of structure and use of transport models.

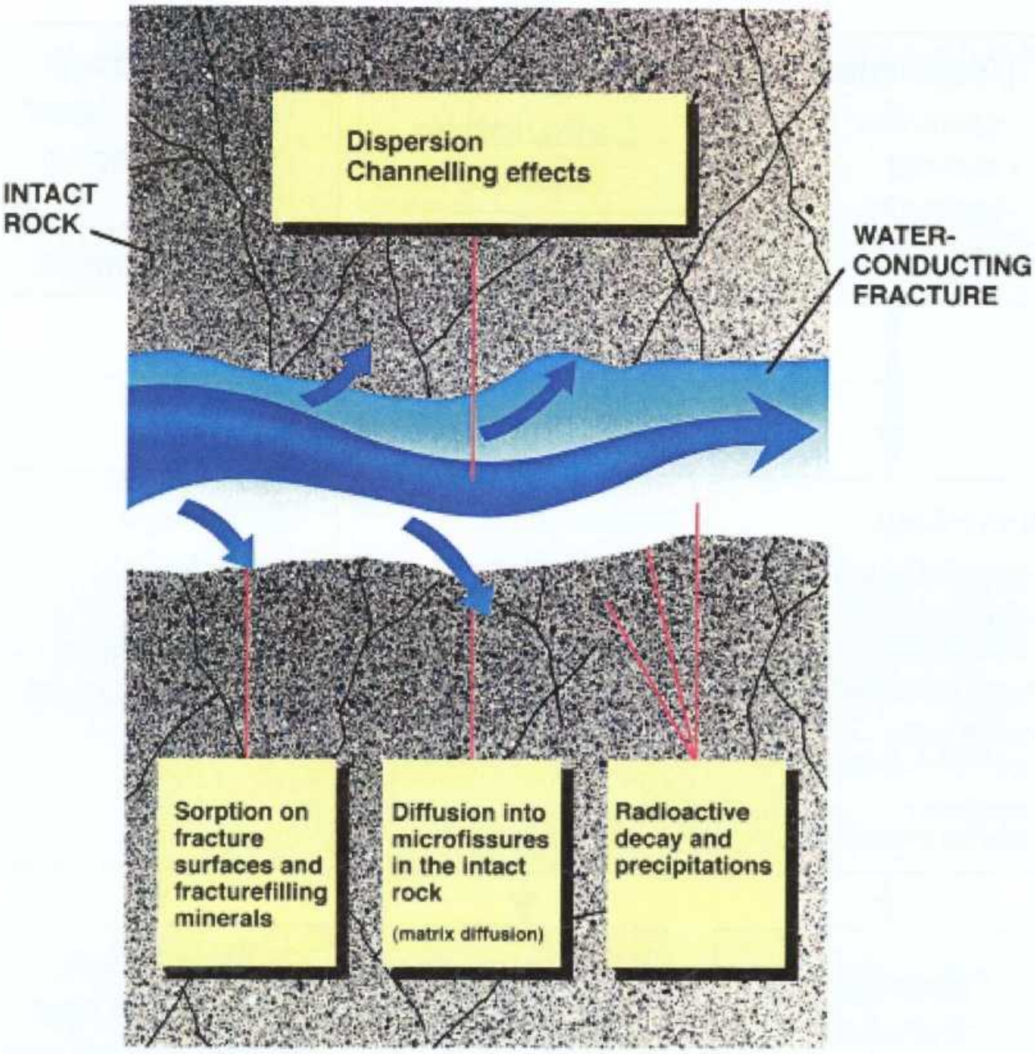


Figure 7-2. Illustration of modelled mechanisms that influence transport of radionuclides in fractured rock (from SKB SR 95).

direct geological equivalent, but refers to the intact rock with microfractures – i.e. fractures in which flow cannot take place.

The requirements on knowledge of data vary between the transport parameters. Only certain retention properties have a great influence on the capacity of the rock to retard released radionuclides for such a long time that they decay. Of the processes modelled today, it is primarily sorption on the surfaces of the microfractures in conjunction with matrix diffusion that has a high retardation potential. The magnitude of the influence of matrix diffusion depends on the interaction between groundwater flow, flow geometry, porosity and diffusivity of the rock matrix and geochemical properties of the groundwater.

There is no clear-cut, generally accepted view of how the transport parameters should be described in detail or related to possible measurements in the field. In the safety assessment's migration calculations, this problem is handled by analyzing different conceptual hypotheses and by (plausibly) conservative choices of parameter values. This entails that information on retention properties obtained in the field is weighed together with knowledge obtained from previous investigations, various research projects or theoretical considerations. This applies in particular to estimates of the "flow-wetted surface" (see below).

7.2.3 Transport in the biosphere

The data requirement for biosphere transport models has already been discussed in Chapter 5, as has the data requirement for land and environment. To a large extent, the data requirement is of a hydrogeological nature. However, in order to be able to assess the flux in different parts, these data need to be supplemented with the transport properties of the soil layers. This is commented on in the present chapter.

7.2.4 Ruling out other transport mechanisms

There is an overall consensus (NEA, 1996) that migration of the radioactive substances that escape from the repository is determined primarily by the transport processes of advection, dispersion, matrix diffusion and sorption. There could, however, also be other conceivable mechanisms such as transport via colloids or via gas. Site-specific data may be needed to show that these other mechanisms can be neglected. Such arguments, based on measured data, were made for example in SKB 91. Site-specific data that are important to know in order to make such judgements have already been mentioned in Chapter 6.

7.2.5 Assessment of changes in groundwater chemistry

Knowledge of migration is also of importance for being able to assess the long-term groundwater chemistry in the repository for different scenarios, which has already been discussed in Chapter 6. It may, for example, be important to know whether changes in the groundwater chemistry in more near-surface groundwaters could influence the groundwater chemistry at depth. Such changes could affect both containment and retention. As a rule, however, such questions can be handled with qualitative information and discussions. In addition to the geochemical information, which is discussed in section 6.5, the retention properties of the rock can also be important information in making such assessments.

7.2.6 Favourable, unfavourable and discriminating factors

In the supplement to RD&D-Programme 92, a number of favourable, unfavourable and discriminating factors are mentioned with a direct bearing on transport properties. Factors rated as *favourable* were a large area/volume ratio in water-bearing fractures and strong chemical sorption capacity along the groundwater's transport pathways in the rock. Factors already listed as unfavourable under the headings "Hydrogeology" and "Geochemistry" (see Chaps. 5 and 6) were rated as *unfavourable*. A factor rated as *discriminating* in the sense that it can occasion abandonment of a site in a site investigation phase was: many closely-spaced water-bearing fracture zones with rapid transport pathways up to the surface.

The identification of transport parameters in the following sections includes all the parameters mentioned above. A further definition of site selection factors can, in other words, be based on the list of parameters in Appendix A:5.

7.3 Properties on a near-field scale

The groundwater chemistry properties that influence the stability of the canister, fuel dissolution, and transport through the bentonite and the rock in the near field have already been commented on in Chapter 6. In summary it can be concluded that groundwater chemistry is of essential importance for the stability of the canister (isolation), as well as of essential importance for retardation in fuel, bentonite and rock. Retardation is dependent above all on the fact that groundwater chemistry influences the solubility of several important radionuclides.

Regarding the importance of the groundwater flow, most source term codes, including Tullgarn/TULL22 (Kjellbert, 1995) and NUCTRAN/COMP23 (Romero et al., 1995) which SKB uses, are based on a very simple description of the groundwater flow in the rock with a plane-parallel fracture that intersects the deposition hole. The geometric and hydrogeological factors that control the leakage are fracture width and groundwater flow in the fracture. Sensitivity analysis with source term codes (SKB, 1992; SKI, 1996) show that the leakage is only dependent on the groundwater flow in a limited interval. Furthermore, an alternative transport pathway could be transport directly to a postulated disturbed zone. If the flow in this is sufficiently great, the leakage will be completely independent of the groundwater flow in the surrounding rock and the leakage via the tunnel will dominate for most groundwater flows (Vieno et al., 1992). The question can, however, be posed as to whether these conclusions would be changed by a more realistic (and less conservative) description of the source term.

In summary it can be concluded that the groundwater flux in the near field is of limited importance for the stability of the canister (influx of corrodants), but in important flow intervals is still of essential importance for retardation in bentonite and near-field rock. According to current (conservative) models, the fracture geometry in the near-field rock is only of limited importance for retardation of leakage, but this assessment may change if more realistic models are used (Andersson et al., 1996).

The above assessments are summarized in the table in Appendix A:6.

Measurement methods

The near-field flows that are needed for source term calculations can be calculated with the hydrogeology models that are used for migration modelling. The distribution of flow paths, as well as the correlation between flow and other transport properties, is less essential, however, which means that the input data on this is in principle subject to less rigorous demands than if the model is only to be used for near-field applications (see Chapter 5). In a detailed characterization phase, however, detailed measurements of the properties of the near-field rock may be highly justified in order to optimize repository design.

7.4 Properties of flow paths

The speed with which solutes are transported in fractured rock is determined by the relationship between transport with the mobile groundwater on the one hand and retardation due to matrix diffusion coupled with sorption in the rock matrix on the other. The properties of the groundwater transport that are of importance in this respect are the groundwater's flow paths, the groundwater flow rate along these flow paths, dispersion, flow porosity and the "flow wetted surface". These parameters can be defined in slightly different ways. They are not independent of each other and they depend on how they are averaged in space. Estimation of these parameters can therefore only be done if the correlations are taken into account. This also means that the methods used to determine the parameters are in some measure the same.

7.4.1 Flow paths, groundwater flow, dispersion and porosity

The transport of solutes through the rock takes place along the groundwater's flow paths. The term "flow paths" is, however, not well defined but is based in individual applications on estimates from a flow model. In the migration models used by SKB in the safety assessment, flow paths and groundwater flow are described as a distribution of streamtubes where each streamtube is represented by groundwater flow, longitudinal dispersion, porosity and length. In each streamtube, transport is described one-dimensionally and can be solved with simple models (e.g. FARF31). With the one-dimensional models, a "flow time" can thereby be calculated for each streamtube for a non-sorbing substance. This flow time is not trivially coupled to the breakthrough time for a sorbing decaying nuclide and is to be regarded as a mathematical quantity. The term "flow time" is thereby unsuitable as a site-specific parameter but can, if need be, used internally in the modelling work.

Owing to the spatial variation of the rock's conductivity, and depending on the applicable boundary conditions, the properties will be different for different streamtubes. It is the distribution of properties that determines the properties of the rock. Several important observations should hereby be made.

In the first place, it should be observed that the properties within a streamtube constitute average values of the varying conditions within the streamtube. The distribution of properties between streamtubes and the dispersivity that has been adapted to a given streamtube are dependent on this scale.

The dispersion within a streamtube is a measure of the flow variations within the streamtube. However, if the streamtube scale is small, the variation in flow between different streamtubes will be a much more important spreading mechanism. Sensitivity analysis and migration models show that dispersion within such streamtubes is of relatively limited importance, especially if the leakage from the source term proceeds over a long period of time (SKI, 1996). In TVO-92 (Vieno et al., 1992), dispersion was not even included in the transport calculations.

The flow porosity in principle determines the groundwater's flow velocity (if the Darcy flow is known). For sorbing substances and for matrix diffusion, however, the flow velocity is of secondary importance. But knowledge of the porosity can be of great importance for being able to interpret tracer tests performed with non-sorbing or weakly sorbing substances.

In order to obtain a reasonable resolution of the flow field, the averaging scale must not be chosen to large. A larger scale entails a reduction in the variability between streamtubes, while dispersion needs to increase to handle the flow variations within the streamtube. Ideally, as high a resolution as possible of the flow field would therefore be needed, after which a suitable scale would be chosen when choosing parameters for the safety assessment. Completely targeted studies of what resolution is needed for meaningful migration calculations have not been carried out. Moreover, the need to determine a suitable scale is overshadowed by the difficulties and uncertainties in determining the groundwater flow rate (and the flow-wetted surface) on smaller scales. A plausible average scale, which was applied in principle in SKB 91, could however correspond to the size of an individual deposition hole, since this is roughly equivalent to the size of the source term.

The one-dimensional streamtube description entails a simplification and does not permit mixing between streamtubes, for example. The model therefore does not work in principle if the flow paths are changed, e.g. as a consequence of future climate change. Nor is it clear how parameters should be weighted in connection with averaging within individual streamtubes. As a rule, however, these difficulties can be handled by a conservative choice of parameter values in the safety assessment.

Alternatives to the description of the flow field as a distribution of streamtubes are being discussed (Ström, 1996). As a rule, these alternatives entail solving the transport problem directly for the flow field that has been calculated with a three-dimensional hydrological model. Since there are different conceptual models for this (see Chap. 5), this also leads to alternative transport models. The need for site-specific data can therefore not be "tailored" to a single model, but must be adjusted so that data can be adapted to all the models intended to be used.

7.4.2 "Flow wetted surface"

Together with groundwater flow, the effective contact area, per volume of rock, between flowing water and the rock is the most important parameter for being able to determine the importance of matrix diffusion. The flow-wetted surface is maximized by the fracture surface area in the rock (which is relatively easy to estimate from structure-geometric data), but is in practice much smaller – only those fracture surfaces with a potential to participate in the transport contribute to the area. Limitations in flow-wetted surface arise due to heterogeneity in the fracture plane (only certain parts of the fracture conduct water) and heterogeneity between fractures (only certain fractures contribute to the flow). This means that there is a correlation between flow distribution, porosity and flow-wetted surface. In other words, the flow-wetted surface is not a parameter that is completely independent of the flow, which means that there is no complete consensus on how it should be parameterized (see Elert, 1996).

Individual values of the flow-wetted surface depend on how it has been defined and how it has been averaged in space and time. The flow-wetted surface can, for example, refer to surface per volume rock or surface per volume water. These are only trivially related via the porosity for simple geometries. Further, the flow-wetted surface per volume of water and the flow velocity are highly interrelated, since both are directly dependent on the flow porosity. However, Moreno and Neretnieks (1993), for example, have shown that the retention properties of a flow path are essentially determined by the ratio between flow-wetted surface per volume of rock and the Darcy velocity. This ratio, which can also be described as the product between flow-wetted surface per volume of water and the flow velocity, is also much more robust against different ways of averaging the different parameters (SKI, 1996).

7.4.3 Evaluation, need for precision and measurement methods

In summary, it can be concluded that determining the exact location of flow paths in the rock is of limited importance for determination of the rock's retention properties. On the other hand, the distribution of the groundwater flow over different flow paths, as well as the flow-wetted surface, are of very essential importance, while dispersion and flow porosity along the flow paths are only of limited importance. All of the parameters mentioned here can, however, be of essential importance for a geoscientific understanding of the site, since for example they influence the possibility of interpreting tracer tests as well as more long-term geochemical changes. Assessments are shown in the table in Appendix A:6.

It follows from the above line of reasoning that site investigations devoted to determining retention properties of flow paths cannot be focused on determining individual well-defined parameters. Information instead needs to be collected that permits interpretation of the broader concepts "flow paths" and "flow-wetted surface" to parameter values for different approaches and descriptions, and on a scale that corresponds to the size of individual deposition holes (see 7.2.1 above).

Interpretation of data to values of streamtube distribution, dispersivity, porosity and flow-wetted surface thereby need to be done in one context and need to be mutually consistent. This notwithstanding, of the information conceivably available for determining these quantities, some has a greater bearing on "flow paths" and other on "flow-wetted surfaces".

The principal source of information on flow paths comes from particle tracks from detailed hydrogeology models. Data needs for such flow paths have already been commented on (see Chap. 5). Opportunities for directly measuring the flow distribution in the rock are limited (see Chap. 5).

The flow-wetted surface can be determined on a micro-scale (lab test on fractures in drill cores, see e.g. Kristallin I, NAGRA, 1994). On the streamtube scale, however, the flow-wetted surface is dependent on the flow distribution on a micro-scale and the flow distribution in the streamtube. There are different approaches for utilizing information on a larger scale, e.g. extrapolation with discrete fracture network models (Geier, 1996) or with channel network models (Gylling et al., 1995), whereby discrete fracture data and measured permeability distributions or flow distributions are utilized.

Attempts are also being made to estimate the flow-wetted surface from fitting of transport models to breakthrough curves in tracer tests, and direct measurements by injection of epoxy followed by breaking-up. Use of geological evidence for matrix diffusion "red colouring" is also being discussed. For further discussion of this, see Elert (1996). However, none of these methods has got beyond the research or conceptual stage, although they are potentially interesting if they could lead to improved means of determining the magnitude of matrix diffusion.

It is worth noting that with the methods available today, both variability and uncertainty regarding flow paths will be considerable. Variability cannot be changed by more measurements, but the uncertainties could possibly be reduced if new methods are developed. It is not clear whether the research that is currently under way will result in practically feasible site investigation methods. But in view of the fact that data on "flow paths" and "flow-wetted surfaces" are currently assumed to be based on extrapolation/upscaling from other models, and in view of how crucial these factors are for retention, efforts should be made to improve data.

7.5 Retention properties of the rock mass along flow paths

Sorption can occur on the surfaces of microfractures inside the rock matrix, i.e. combined with matrix diffusion, and on larger fracture surfaces in direct contact with the flowing water. SKB's migration models (FARF31) mainly deal with sorption in the matrix and neglect the sorption directly on the macrofractures. To be able to determine the importance of sorption in the rock matrix, information on the sorption as well as on the diffusivity and porosity of the rock matrix is needed. The values used must be representative of the actual flow paths.

7.5.1 Sorption

In the migration models in the safety assessment, the sorption of radionuclides dissolved in the groundwater is described with the sorption coefficient Kd, which designates the distribution of radionuclides between the water and the rock. In principle, Kd values are dependent both on groundwater chemistry (mainly redox) and mineralogy (see section 6.4). This is dealt with by choosing conservative values for the groundwater chemistry.

7.5.2 Matrix diffusivity, matrix porosity and maximum penetration depth

Matrix diffusion is also determined by the properties of the matrix (diffusivity and porosity). Moreover, these properties can be assumed to decline at a certain distance from the fracture, so that models also as a rule contain a stipulated maximum penetration depth, which is a conservative estimate of how much of the rock matrix is accessible for diffusion.

7.5.3 Evaluation, measurement methods and need for resolution

Sensitivity analyses with migration models (see e.g. Vieno et al., 1992 or SKI, 1991) show that sorption data, matrix diffusivity and matrix porosity are essential for determination of the retention properties of the rock. However, the requirement on precision is much lower than for the ratio of flow to flow-wetted surface (or equivalent parameters). The resultant retention is in principle only dependent on the square root of the former parameters. The maximum penetration depth is of limited importance, since in most cases even if very conservatively small values of the penetration depth are specified, they are nevertheless generally so large that no additional effect would be achieved if larger values were assigned. The density of the rock mass is included in the sorption formulas, but the variation of the density between different rock types is nearly negligible in this context, so the information is only of limited importance.

Generic data exist today of the transport parameters that are based on the results of previous investigations. Without anticipating the results of the investigations that are in progress, for example on Äspö, it nevertheless appears evident that *site-specific data should be measured* for sorption, porosity, diffusivity, penetration depth and flow-wetted surface.

The assessments are also summarized in the table in Appendix A:6.

A serious problem in characterizing the rock along flow paths is that the exact location of the flow paths is not known, and furthermore that the drilling technique can determine what can be seen in the fractures. Variability in the fracture plane can be considerable and really needs to be characterized. It is therefore not a simple matter to obtain "representative data".

The traditional way to obtain sorption data is to measure sorption coefficients, Kd values, for essential radionuclides and representative minerals. Since sorption is of greatest importance in conjunction with matrix diffusion, importance has been attached to using rock-forming minerals, e.g. a mixture of plagioclase, biotite, potash feldspar and quartz (crushed rock). From a large number of measurements, a careful selection of representative Kd values is made.

Measuring Kd in situ by means of e.g. tracer tests or CHEMLAB is hardly necessary for the safety assessment, other than to verify that laboratory values are usable (validation). On the other hand, the sampling technique itself is of course essential, for example flushing-out of clay minerals in conjunction with drilling can make it impossible to obtain representative samples. If clay minerals are much more common than is believed, it may be a pity to miss that capacity for sorption.

Diffusivities and porosities are measured on sawed-out slices of the rock and maximum diffusion depth is estimated from e.g. analogue studies. It has not been considered necessary to take the samples from the site that is the object of a specific safety assessment; rather, the results should be generally applicable where conditions are similar in our country (granitic rock). Against that background, it could be asserted that we already know enough, especially considering how difficult it is to obtain good values of other essential parameters such as flow-wetted surface. On the other hand, it is not impossible that the body of data could actually be improved quite a bit by means of a targeted campaign on a given site. Development in this area is being pursued on Äspö.

If diffusion parameters could be measured in situ, there would be no question as to whether the sample had been altered structurally in conjunction with sampling (release of stress). No such technique that is practically useful is available today. The aim should therefore be to take samples for analysis in the laboratory after first having shown that the technique yields a relevant result.

There are thus established methods for measuring Kd, matrix diffusivity and matrix porosity in the laboratory. But technology has progressed, so it is a good idea to review the available options and choose methods that are simple to use but still give good enough results. Diffusion is an example of this. Current technology is good but slow. With newer methods, if they prove reliable, it will be possible to measure more samples in a shorter time.

Measuring the constants that are needed to describe the formation of surface complexes is exceedingly difficult. It involves measuring chemical changes caused by changes in concentration on the surfaces of a suspended mineral in an aqueous solution. The changes are small and low concentrations of impurities tend to disturb the measurement by for example "settling on the surfaces". There are examples where it has taken a year for scientists to manage to make successful measurements a single nuclide on a single simple mineral. Then it has been a question of painstaking work in a controlled atmosphere (glovebox) and with extremely pure synthetically produced mineral samples. There are also other discouraging examples where attempts have finally met with failure due to the fact that the mineral surface (feldspar) slowly reacted in the solution, rendering measurement impossible.

Surface complexation is an excellent method for demonstrating an understanding of the sorption mechanisms, but it is far from being an acceptable alternative to the use of Kd values. In other words, Kd values should not be replaced with surface complexation constants in the safety assessment. It may be possible one day, but it would be unwise to promise anything.

NAGRA is in the process of testing a method of assigning fractures in the rock to different classes with different retention properties. SKB is involved in this development work via Äspö. It is possible that this will succeed. For it to work, there should not be too much variation within a class. The important thing is that the range of variation in retention parameters within a class does not greatly exceed the difference between different classes.

7.6 Transport parameters in soil layers/receptors

For biosphere modelling there is a need to know the retention properties in the soil layers in order to be able to calculate flux and retardation in various receptor compartments. Information is thereby needed on water flux (from hydrological or hydrogeological analysis, see Chap. 5), flow porosity, sorption properties and microbiological activity that can further contribute to retardation or accumulation. Flow porosity is of limited importance for biosphere modelling, but can be important for short-term analysis of other environmental consequences from the deep repository. Water flux, sorption properties and microbiological activity that can contribute to accumulation are of essential importance for both biosphere modelling and assessment of more short-term "traditional" environmental consequences. The assessments are shown in the table in Appendix A:6.

7.7 Supporting data

7.7.1 Geochemical characterization of fracture filling, wall rock and groundwater

There ought to be a number of different measures that could be undertaken on a selected site to underpin the safety assessment that has already been carried out. One suggestion is to go through and analyze, in both water and minerals, the trace elements that occur and chemically resemble radionuclides, such as U, Th, Ra, Se, Mo, Sn, Rb, Zr, Ni, Sr, Cs, lanthanides, or other important components from a repository, for example Cu. For this to be meaningful, it must naturally be practically possible to analyze the element in question. Long tables with N D (Not Detected) are no help to anyone. But if the measurements are truly successful, they can be used to a) check calculations of solubility and b) support conclusions regarding the retention of radionuclides in the rock (e.g. via sequential extraction).

Considerable efforts have been made to enable retention via co-precipitation to be used for the migration calculations in the safety assessment, but it is not easy. Experiments, e.g. co-precipitation with calcite, have not been particularly successful, and the models that exist are somewhat controversial. Another difficulty consists in being able to show that the precipitate is not dissolved at a later stage or changed with time so that it eventually "rejects" the co-precipitated radionuclide, for example when amorphous iron(III)hydroxide is converted to crystalline goethite. It must also be possible to show that precipitation really takes place in some stage of the radionuclide transport. Thus, it is not possible to utilize co-precipitation today in the safety assessment's calculations of radionuclide transport in the rock. But in order to interpret observations of solubility and sorption of tracers correctly, it is necessary to know whether solid solutions have been formed in the minerals. This can be achieved by revealing states of oversaturation in the water and signs of precipitation in the fracture minerals.

The possibility of using geochemical data, e.g. "red colouring of flow paths", as an indication of matrix diffusion and thereby as a possible way to measure the flow-wetted surface is being discussed, but there is no developed methodology for this today (see e.g. Elert, 1996).

Evaluation, measurement methods and desirable data:

In summary, it can be concluded that geochemical characterization of fracture filling, wall rock and groundwater is of essential importance for a geoscientific understanding of the rock – and thereby indirectly for justifying the plausibility of chosen transport models. The information could also be directly useful for interpreting important transport properties, such as flow-wetted surface, but since methodology for this is not established, the information is judged today to be of limited importance for this purpose. The assessments are also shown by the table in Appendix A:6. (See also discussion in Chaps. 2 and 6.)

Trace element analyses should be performed on the samples from the 20–30 types of fracture fillings with associated wall rock and 10–20 reference samples of fresh, unaltered rock as mentioned above in connection with determination of the retention properties of the rock for the safety assessment. It is then of the utmost importance that analyses be available of equivalent substances in water that has run through the sampled fractures. This relationship must be clear for it to be possible to interpret the results in a meaningful way. To trace the influence of co-precipitation, special attention should be given to calcite, iron(III) and manganese(IV) minerals.

7.7.2 Tracer tests

In principle, tracer tests should be important sources of indirect information on the retention properties of the rock. For this reason, Appendix A:6 states that breakthrough curves from tracer tests are essential for being able to determine the retention properties of the rock as well as for a geoscientific understanding.

Unfortunately, though, tracer tests actually performed (Stripa, Äspö, etc.) have only been able to be used to a limited extent to indirectly estimate important properties of the migration models such as flow distribution and actual flow-wetted surfaces, even though they have been able to be used to justify the plausibility of the chosen model and model parameters. In order to make tracer tests truly useful in the site investigation programme, technology and evaluation methods for them need to be developed.

There are good reasons why tracer tests have so far only been utilized to a limited extent. Some of them are technical, but the main problem is that tracer tests that are truly sensitive to the flow-wetted surface take a long time to perform. The value of conducting tracer tests in a limited portion of the rock, when predictions are needed of a large portion of the rock, can also be questioned.

By more active design, by not beginning tests too late and by allocating resources for evaluation, it is nonetheless possible that tracer tests could be developed into a more active instrument for site investigations. The experience that has now been gained within the Äspö Project (LPT2, TRUE etc.) should be compiled to arrive at a programme for tracer tests in site investigations.

7.7.3 Groundwater chemistry and estimation of colloids, gas, etc.

Data needs for this have already been commented on in Chapter 6.

8 Conclusions

This document has identified and evaluated geoscientific parameters that are of importance to know in order to be able to carry out performance and safety assessments of a deep repository for spent nuclear fuel, based on the information that can be obtained from a site investigation. The document also discusses data needs for planning and design of the rock works and for description of land and environment. The document can thereby serve as a point of departure for:

- a description of measurement, interpretation and analysis methods,
- a description of how data are analyzed in safety and performance assessments and the need for feedback to the site investigation programme,
- a discussion of more precisely defined site selection factors,
- a discussion of in what logical sequence different measurements need to be carried out with regard to both the need for input data and influence on other measurements.

Together, this information should comprise an essential body of background material for the planning of a geoscientific site investigation programme. It should also be pointed out that the present document may need to be revised, for example based on experience from SR 97. This notwithstanding, it may also be used in its current form for the necessary planning.

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APPENDIX A:X

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Regarding evaluation of the importance of parameters

The importance of a parameter for the performance of the deep repository is evaluated in Appendices A:1 – A:6 as follows:

(E) Essential importance

(L) Limited importance

(Empty box) No importance

It should be noted that the table is a simplified and abridged presentation of the contents of the report.

The evaluation is mainly based on conventional assessments of the importance of the information for a deep repository, in some cases on the subjective judgements of the authors and consulted experts.

There is no direct relationship between the importance of a parameter and the scope and accuracy with which it is determined during a site investigation.

The list of parameters is for the most part applicable to all phases of the siting, construction and operation of the deep repository. Many parameters are, however, only dealt with during one or a couple of these phases, while other parameters can be determined with increasing accuracy as increasingly detailed investigations are made.

The fact that a parameter is evaluated with (E) or (L) in the table means that in at least one of the investigation phases it is of essential or limited importance for the performance etc. of the deep repository to determine the parameter.

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

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Influence, importance / DISCIPLINE – parameters	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
GEOLOGY																
Topography																
Topography			E					E							E	
Soil layers																
Soil types																
Thickness of soil cover								L		L	L			L	L	
Soil type distribution										L				L	L	
Soil type description										L				L	L	
Soil										L				L	L	
Bottom sediment								L		E				L	L	
Indication of neotectonics			E												E	
Lithology																
Lithological structure																
Rock type distribution			L						L		E	E			E	
Xenoliths															E	
Dikes											E	E			E	
Contacts											E	E			L	
Age															L	
Ore potential – industrial minerals				E							E				E	
Rock type description																
Mineralogical composition			L						L		E	E	E		E	
Grain size			L								E	E			L	
Mineral orientation															L	
Microfractures									L						L	
Density															L	
Porosity									L						E	
Susceptibility/gamma radiation etc.															L	
Mineralogical alteration/weathering			L						L		E	E			E	
cont'd. on next page																

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

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Influence, importance / DISCIPLINE – parameters	Long-term performance and radiological safety										Design			Other environ-mental aspects	Geos. under-standing	Note
	Isolation				Retardation					Biosphere						
	Canis-ter	Bento-nite	Rock	Intru-sion	Fuel	Canis-ter	Bento-nite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
Structural geology																
Plastic structures																
Folding															E	
Foliation			L									E			E	
Lineation															E	
Shear zones			L									E			E	
Veining															E	
Age															L	
Brittle structures																
Faults	E	E	E					E	L							
Fractures (fracture zone)	(E)	(E)	E					E	E							
Age																
Properties of discontinuities (Brittle and plastic structures of mechanical importance)																
Regional and local discontinuities																
Position	E	E	E					E	L		E	E			E	
Orientation			E					E			E	E			E	
Length			E					E			E	E			E	
Width			E					E			E	E			E	
Movements (size, direct., age)			E								E	E			E	
Properties																
number of fracture sets			E								E	E			E	
spacing			E								E	E			E	
block size			E								E	E			E	
fracture roughness			E								E	E			E	
fracture filling (fracture mineral)			E						L		E	E			E	
altertion/weathering			E						L		E	E			E	
cont'd. on next page																

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

Influence, importance / **DISCIPLINE – parameters**	**Long-term performance and radiological safety**										**Design**			**Other environ-mental aspects**	**Geos. under-standing**	**Note**
	Isolation				**Retardation**					**Biosphere**						
	Canis-ter	**Bento-nite**	**Rock**	**Intru-sion**	**Fuel**	**Canis-ter**	**Bento-nite**	**Rock**			**Layout**	**Construct. analysis**	**Working environm.**			
								Gw flow	**Retention**							
Local minor discontinuities																
(data for stochastic/																
deterministic description)																
Position			E					E			E	E			E	
Orientation			E					E			E	E			E	
Length			E					E			E	E			E	
Width			E					E			E	E			E	
Movements (size, direct.)			E												E	
Properties															E	
number of fracture sets			E					L	L		E	E			E	
spacing			E					L	L		E	E			E	
block size			E					L	L		E	E			E	
fracture roughness			E								E	E			E	
frature filling (fracture mineral)			E					L	L		E	E			E	
alteration/weathering			E					L	L		E	E			E	
Individual fractures (Data for																
stochastic description)																
Spacing (different sets)			E					E	E			E			E	
Orientation			E					E	E		L	L			E	
Persistence (length)			E					E	E			L			E	
Contact pattern			E					E	E			L			E	
Aperture width			E					L	L			E			E	
Roughness			E									E			E	
Filling (fracture mineral)			E					L	L			E			E	
Alteration/weathering			E						L			E			E	

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

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Influence, importance / DISCIPLINE – parameters	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
ROCK MECHANICS																
Discontinuities																
Geometry of discontinuities and geological parameters	E	E	E					E			E	E			E	
Mech. properties, indiv. fractures in diff. rock masses																
Deform. properties, normal dir.	E	E	E					L			E	E			E	
Deform. properties, shear dir.	E	E	E					L			E	E			E	
Shear strength (e.g. fi, c, JRC, JC)	E	E	E					L			E	E			E	
Mech. properties, intact rock in different rock masses																
Young's modulus	E	E	E					L			E	E			E	
Poission's number	E	E	E					L			E	E			E	
Compressive strength	E	E	E					E			E	E			E	
Tensile strength	E	E	E					E			E	E			E	
Indentation index, DRI, wear index											L	E				
Blastability											L	E				
Mech. properties of different rock masses																
Young's modulus	E	E	E					L			E	E			L	
Poisson's number	E	E	E					L			E	E			L	
Rock classification (Q, RMR)			E								E	E				
Dynamic prop. vel. – compr. wave	E	E	E												E	
Dynamic prop. vel. – shear wave	E	E	E												E	
Strength – distribution	E	E	E					E			E	E			L	
Density and thermal properties																
Density	L	L	L								L				L	
Coefficient of thermal expansion	E	E	E								E					
Thermal conductivity	E	E	E								E					
Specific heat	E	E	E								E					
Boundary conditions/ supporting data																
Stress distribution	E	E	E								E	E			E	
Future loads	E	E	E					E							E	
Observ. deformations, seismics			E								E	E			E	

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation
on page 115)

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Influence, importance / DISCIPLINE – parameters	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
THERMAL PROPERTIES																
Properties of the rock																
Thermal conductivity – rock	E	E	E					L			E				E	
Heat capacity – rock	E	E	E					L			E				E	
Thermal expansion	E	E	E								E				E	
Temperature																
Temperature, rock and groundwater	L	L		L	L			L			E				E	
Thermal boundary conditions and gradient	L	L		L	L			L							E	

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

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DISCIPLINE – parameters / Influence, importance	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
HYDROGEOLOGY																
Deterministically modelled discontinuities																
Geometry – see geological model			E					E	E		E	E	E		E	
Permeability dist./connectivity	L	L	E					E	E		E	E	E		E	
Flow porosity									L			L			E	
Storage coeff.															L	
Stochastically modelled discontinuities and fractures plus rock mass																
Statistical discontinuities – see geo	L	L	L					E	E						L	
Permeability dist./connectivity	L	L	L					E	E		E	E	E		E	
Flow porosity	L		L						L						E	
Storage coeff./Compressibility															L	
Groundwater properties																
Salinity								E							L	
Temperature								L								
Properties of soil layers																
Identification of receptors										E				E	L	
Meteorological/Hydrological data								L		E				E	E	
Conductivity, thickness, porosity								L		E				E	L	
Boundary conditions/ supporting data																
Groundwater pressure/head								E			E	E	E		E	
Measured groundwater flow								E							E	
Breakthrough curves								E							E	
Recharge/discharge areas								L		E					L	

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

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DISCIPLINE – parameters / Influence, importance	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
CHEMISTRY																
Groundwater chemistry																
Eh	E				E				E						E	
pH	L	L			L				E						E	
Na		E					E		E						E	
K		E													E	
Ca		E					E		E						E	
Mg		E													E	
HCO_3	L				L				E						E	
SO_4	L								L						E	
Cl	E						E		E					L	E	
Fe	E				E				E						E	
Mn									L						E	
U													E		E	
Th															E	
Ra															E	
Si		L													E	
Al		L													E	
Li															E	
Cs															E	
Sr															E	
Ba															E	
HS	E				E				E						E	
I															E	
Br															E	
F															E	
DOC	L														E	
TDS		E													E	
O-18 (i H_2O)															E	
H-2 (i H_2O)															E	
C-13 (i DIC)															E	
C-13 (i DOC)															E	
S-34 (i SO_4)															E	
cont'd. on next page																

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

Influence, importance / DISCIPLINE – parameters	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
O-18 (i SO_4)															E	
S-34 (i HS)															E	
Sr-87 / Sr-86															E	
T															E	
C-14 (i DiC)															E	
C-14 (i DOC)															E	
U^{234} / U^{238}															E	
HA / FA									E						E	
NO_3	E															
NO_2	E															
NH_4	E															
HPO_4	L								L							
N_2									E						E	
H_2	L								E						E	
CH_4	L								E						E	
CO_2									E						E	
Ar									E						E	
He									E						E	
Radon													E			
Bacteria	L								E						E	
Colloids									E							
O_2																
XE isotopes															L	
Kr isotopes															L	
Cl-36															L	
He-3															L	
He-4															L	
Trace metals, other															L	

Geoscientific parameters (sorted according to disciplines) and their importance for the safety performance of the repository, facility design, etc.

E = Essential importance
L = Limited importance
(see note on evaluation on page 115)

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Influence, importance DISCIPLINE – parameters	Long-term performance and radiological safety										Design			Other environmental aspects	Geos. understanding	Note
	Isolation				Retardation					Biosphere						
	Canister	Bentonite	Rock	Intrusion	Fuel	Canister	Bentonite	Rock			Layout	Construct. analysis	Working environm.			
								Gw flow	Retention							
TRANSPORT PROPERTIES																
Near-field scale																
Groundwater chemistry – see chemistry data	E	E			E		E		E							
Groundwater flow	L						E		E							
Fracture aperture, geometry	L						L		L							
Properties, flow paths																
Flow paths									L	E					E	
Groundwater flow paths									E						E	
Dispersion									L						E	
Flow porosity									L						E	
Flow-wetted surface									E						E	
Intact rock along flow path																
Sorption data (Kd)									E						E	
Matrix diffusivity									E						E	
Matrix porosity									E						E	
Max. penetration depth									L						L	
Density of rock matrix									L						L	
Soil layers																
Water flux										E				E		
Flow porosity										L				L		
Sorption properties										E				E		
Biological activity										E				E		
Supporting data																
Breakthrough curves									E						E	
Chemical analysis, fracture filling									L						E	
Chemical analysis, wall rock									E						E	
Groundwater chemistry – see chemistry									E						E	

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April 1998

ISSN 0284-3757
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