R-03-09

Transport properties site descriptive model

Guidelines for evaluation and modelling

Sten Berglund, WSP Environmental

Jan-Olof Selroos, Svensk Kärnbränslehantering AB

April 2004

Svensk Kärnbränslehantering AB
Swedish Nuclear Fuel
and Waste Management Co
Box 5864
SE-102 40 Stockholm Sweden
Tel 08-459 84 00
+46 8 459 84 00
Fax 08-661 57 19
+46 8 661 57 19

ISSN 1402-3091
SKB Rapport R-03-09

Transport properties site descriptive model

Guidelines for evaluation and modelling

Sten Berglund, WSP Environmental

Jan-Olof Selroos, Svensk Kärnbränslehantering AB

April 2004

Abstract

This report describes a strategy for the development of Transport Properties Site Descriptive Models within the SKB Site Investigation programme. Similar reports have been produced for the other disciplines in the site descriptive modelling (Geology, Hydrogeology, Hydrogeochemistry, Rock mechanics, Thermal properties, and Surface ecosystems). These reports are intended to guide the site descriptive modelling, but also to provide the authorities with an overview of modelling work that will be performed.

The site descriptive modelling of transport properties is presented in this report and in the associated "Strategy for the use of laboratory methods in the site investigations programme for the transport properties of the rock" /Widestrand et al, 2003/, which describes laboratory measurements and data evaluations. Specifically, the objectives of the present report are to:

- Present a description that gives an overview of the strategy for developing Site Descriptive Models, and which sets the transport modelling into this general context.
- Provide a structure for developing Transport Properties Site Descriptive Models that facilitates efficient modelling and comparisons between different sites.
- Provide guidelines on specific modelling issues where methodological consistency is judged to be of special importance, or where there is no general consensus on the modelling approach.

The objectives of the site descriptive modelling process and the resulting Transport Properties Site Descriptive Models are to:

- Provide transport parameters for Safety Assessment.
- Describe the geoscientific basis for the transport model, including the qualitative and quantitative data that are of importance for the assessment of uncertainties and confidence in the transport description, and for the understanding of the processes at the sites.
- Provide transport parameters for use within other discipline-specific programmes.
- Contribute to the integrated evaluation of the investigated sites.

The site descriptive modelling of transport properties, and hence the guidelines in this report, involve two main categories of parameters:

- ***Parameters that characterise the retention properties of geologic materials.*** These parameters quantify the diffusion and sorption properties of intact and altered rock, fracture coatings and fracture-filling materials, and are described within the framework of the 3D geometric models devised by Geology.
- ***Parameters that characterise solute transport along flow paths (flow-related transport parameters).*** These parameters include the "*F*-parameter" and "water travel time", t_w, and parameters that account for spatial variability in diffusion and sorption. The flow-related parameters are obtained by means of particle tracking simulations in groundwater flow models.

Contents

1 Introduction

1.1 Background

The Swedish Nuclear Fuel and Waste Management Company (SKB) is responsible for the handling and final disposal of the nuclear waste produced in Sweden. The process of developing a solution for final disposal of the waste has reached the stage of finding a suitable site for a deep repository /SKB, 2001a/. Site Investigations are an important part of the work conducted to site the deep repository. SKB has presented a general investigation and evaluation programme /SKB, 2000/, and a more detailed description of the general programme for the Site Investigations /SKB, 2001b/. In 2002, SKB commenced Site Investigations at two potential sites for a deep repository, Forsmark and Simpevarp. These investigations, which will be carried out in different stages, shall provide the broad knowledge base required to evaluate the suitability of the investigated sites for the repository.

The development of Site Descriptive Models is an essential part of the Site Investigations. The Site Description should cover the geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties and the surface ecosystems of the site /SKB, 2001b/. The site descriptive modelling provides a framework for data interpretation and evaluation, as well as for assessment and presentation of the geoscientific understanding of the investigated site. It involves the whole process from data deliveries from the sites to model deliveries to the "end users" Design and Safety Assessment. Site Descriptive Models are produced within each of the subject areas (disciplines) listed above; however, strong emphasis is to be put on interdisciplinary consistency and integrated evaluation /Andersson, 2003/.

SKB has developed a procedure for Quality Assurance (QA) of the Site Investigations; for an overview, see /SKB, 2000/. Essentially, the aim of the QA procedure is to ensure that the correct work is done, and that the work is done correctly. Programmes and operating plans are the instruments used to secure that the correct work is done, whereas Activity Plans (AP) control how the work is done. Activity Plans usually refer to Method Descriptions (MD) that specify SKB's general requirements upon the methods in terms of working procedures, management of data, and presentation and required accuracy of results. Method Descriptions have been (or will be) established for all methods that will be used to measure and evaluate field and laboratory data during the Site Investigations.

The process of site descriptive modelling is described in a series of reports, see Section 1.2.2, one report for each modelling discipline or subject area and an additional report describing the integrated evaluation. These reports present strategies for the development of Site Descriptive Models, providing the link between data, collected and presented in accordance with Method Descriptions, and the models that constitute the site description. The current document presents the strategy for the development of the site descriptive model of the transport properties of the rock.

1.2 Strategy for site descriptive modelling

1.2.1 Requirements

The Site Descriptive Models that are produced during the Site Investigations should be multidisciplinary interpretations that express the geoscientific understanding of the investigated sites at a given time and provide a basis for further analyses within Design and Safety Assessment /SKB, 2001b/. The following general requirements apply for the site descriptive modelling strategy /Andersson, 2003/:

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

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

The Strategy should ease interaction with Safety Assessment, Site Investigations and Design, by providing the information needed at different stages, and be able to handle feedback from these activities. Specifically, the strategy shall also guide in establishing when the Site Evaluation, based on investigations from the surface, has fulfilled the characterisation phase to a sufficient degree that the sites are comparable, thus forming a basis for decision on siting the deep repository.

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

The strategy should make use of both past experiences and experiences to be gained during the site investigation. It needs to be adaptable to coming needs and experiences and could thus not be overly detailed.

It should be noted that the strategy, including the present document, will be updated when needed. For example, updates could be motivated by experiences from the modelling work, and by results from ongoing research.

1.2.2 Modelling process

The site investigation programme and the site descriptive modelling have a discipline-specific structure with the disciplines Geology, Rock Mechanics, Thermal Properties, Hydrogeology, Hydrogeochemistry, Transport Properties and Surface Ecosystem. Parts of the site descriptive modelling are performed individually by the different disciplines, but the modelling work will to large extent be based on a close cooperation and integration between the disciplines. The process of developing a Site Description is illustrated in Figure 1-1. The Site Descriptive Model consists of a description of the geometry and properties of the identified geological units at the site (rock and soil units, larger structures). This model, together with the databases, constitutes the backbone of the Site Description.

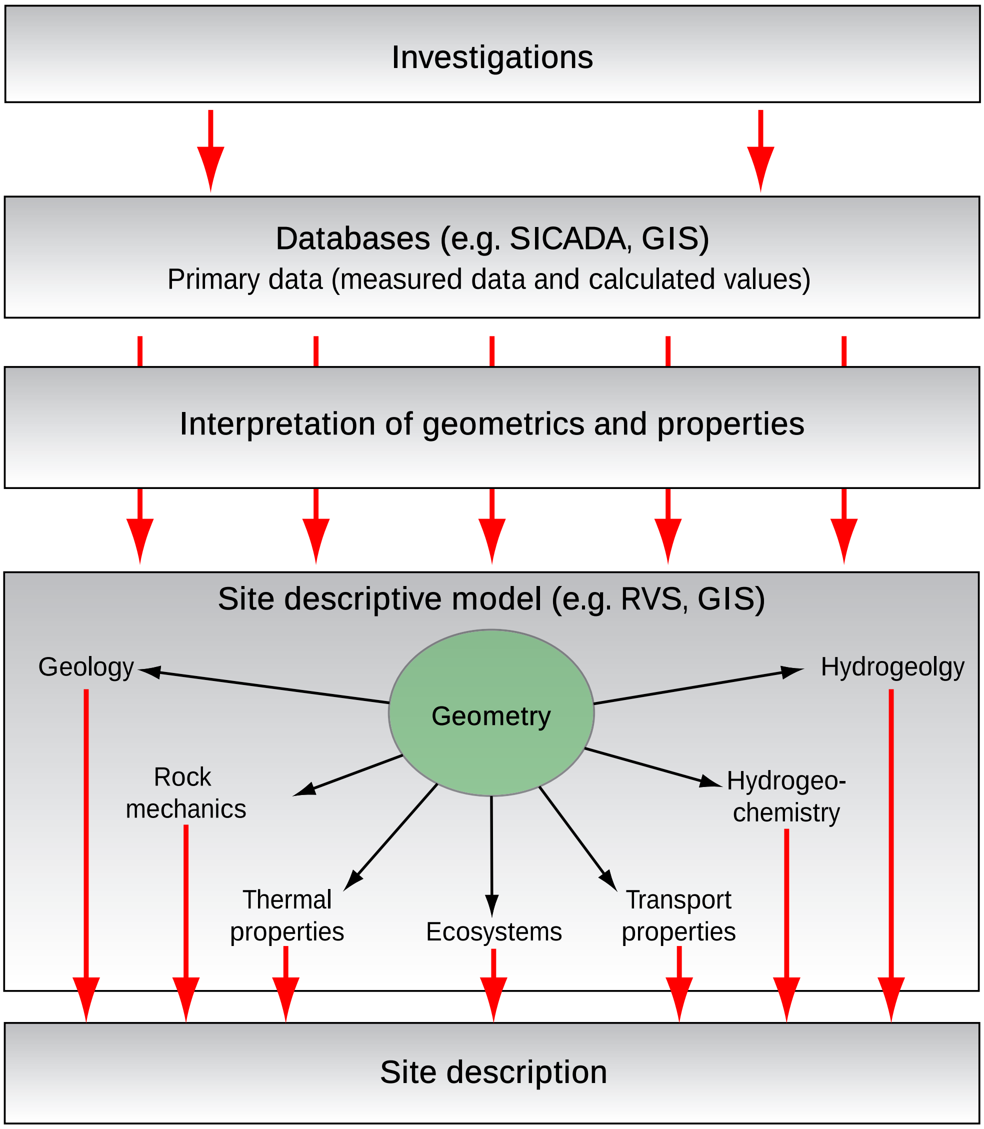


***Figure 1-1.** Development of a site description. The primary data is collected in a database. Data is interpreted and presented in a Site Descriptive Model, which consists of a description of the geometry and different properties of the site.*

The site descriptive modelling concerns assignment of parameter values, which, as indicated in Figure 1-1, are to be described within a common geometric framework. The modelling process may be divided into a number of different steps or components, see Figure 1-2 and the description given by /Andersson, 2003/. The primary data is produced by the investigation organisations at the sites and is stored in SKB's databases. Although this is not a responsibility of the participants in the site descriptive modelling projects, interaction is necessary in order to assure that the required types and amounts of data will be available when needed.

In the site descriptive modelling process, the primary data is evaluated and transformed into the context of the three-dimensional description of the site. The primary data to be used in the development of a new or updated model version (or an alternative model) is extracted from the databases, and is then evaluated within each discipline. This *evaluation of primary data* includes both quality control and interpretations aiming to provide data and models that can be used in the three-dimensional description. The next main step, *three-dimensional modelling*, concerns estimations of geometry and parameters in three dimensions. The basis for this modelling is a geometrical framework provided by Geology. The three-dimensional modelling also includes interdisciplinary assessments of the confidence and uncertainty in the description.

These main steps are followed by an *overall confidence assessment*, involving a comparison between the new model and previous models. The Site Descriptive Model is then delivered to the users, primarily Design and Safety Assessment. It is emphasised that the development of a model may be an iterative process. The users' assessment of the significance of the uncertainties and the modellers' assessment of the prospects of reducing the uncertainties by additional measurements are important for the decisions on whether to perform additional loops in the modelling sequence.

The site descriptive modelling is described in a number of discipline-specific reports and a report describing the integrated evaluation:

- Geological site descriptive model – a strategy for the model development during site investigations /Munier et al, 2003/,
- Hydrogeological site descriptive model – a strategy for the development during site investigations /Rhén et al, 2003/,
- Hydrogeochemical site descriptive model – a strategy for the model development during site investigations /Smellie et al, 2002/
- Site investigations. Strategy for rock mechanics site descriptive model /Andersson et al, 2002/,
- Thermal site descriptive model – a strategy for the model development during site investigations /Sundberg, 2003/,

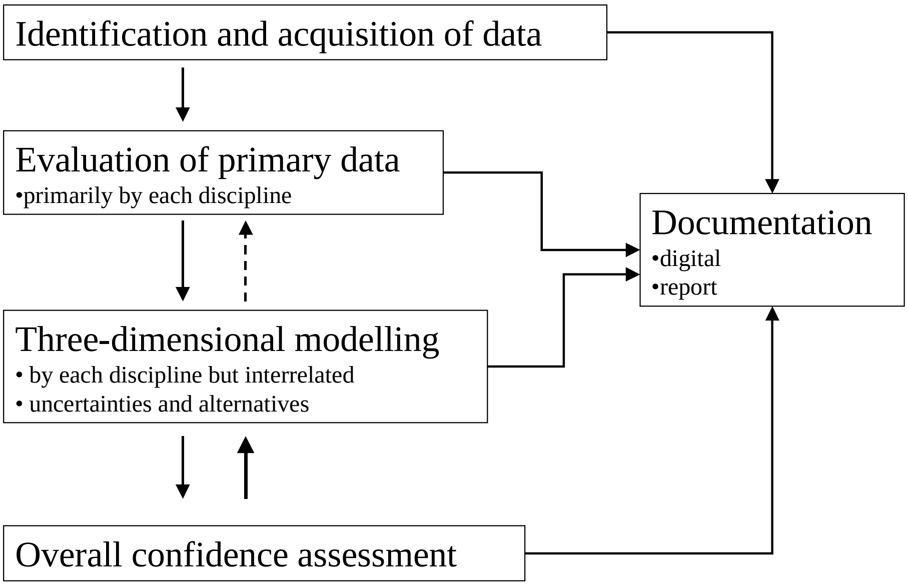


Figure 1-2. *The site descriptive modelling process /from Andersson, 2003/.*

- Ecological site descriptive model – a strategy for the development during site investigations /Löfgren et al, 2003/,
- Transport properties site descriptive model – guidelines for evaluation and modelling (this document),
- Site descriptive modelling – strategy for integrated evaluation /Andersson, 2003/.

These reports are intended to guide the site descriptive modelling and to give external reviewers and authorities an overview of how the modelling will be performed.

1.3 Basic modelling concepts

The Site Description should include descriptions in both *Regional scale* and *Local scale* /SKB, 2001b/. The Local model domain is expected to cover an area of 5–10 km^2. The depth of the modelled Local scale domain is approximately 1000 m. The description in Local scale must be detailed enough for the analyses to be performed within Design and Safety Assessment. The Regional model domain covers a large area around the Local domain. The Regional description is less detailed than the one in Local scale, but it should be sufficiently detailed to provide an overall understanding of the geoscientific (primarily geological and hydrogeological) conditions in the area. An important purpose of the Regional description is to provide input data for Regional scale groundwater flow models that are used to define boundary conditions for the more detailed Hydrogeological models in Local scale.

An essential part of the site descriptive modelling is to determine parameter values for different elements/volumes within 3D geometric models that represent the Local and Regional model domains. The subdivision of a model domain into different volumes is based on differences in properties that are important for Design and Safety Assessment. In practice, the geometric modelling will to a large extent be determined by the geological interpretation of the investigated domain. The smallest volume within a geometric model is called a *unit*. As a result of the interpretations made by the different disciplines, basic geological units with similar properties may be grouped into a *domain*.

Below, a few key terms related to site descriptive modelling in general, and geometric and geological modelling in particular, are defined. The definitions are based on those given by /Munier et al, 2003/, who, however, provide more detailed descriptions and some additional terminology.

Site description (Sw: platsbeskrivning): A site description consists of 2D (GIS) and 3D (RVS, Rock Visualisation System) models, connected to databases containing data from site investigations (SICADA, SIte ChAracterisation DAtabase, and SDE, a GIS database), and a written description (Technical Report), which explains in detail the modelling process, indicates sources of error, gives estimates of uncertainties, and makes recommendations for further investigations.

Parameter (Sw: parameter): This term is used in a very wide sense in the SKB Site Investigations context, such that it includes all characteristics, features and properties, irrespective of whether they are quantifiable and measurable or not. In the present report, however, the term almost exclusively refers to quantifiable characteristics, and the term “parametrisation” implies that numerical values are assigned to different objects in a model.

Geological model (Sw: geologisk modell): A geoscientific model that shows the geometries of superficial deposits, rock units, deformation zones, etc, together with their characteristic parameter values. Specifically, a geological model for the bedrock consists of a combination of a lithological model and a structural model.

Deformation zone (Sw: deformationszon): An essentially 2D structure (a sub-planar structure with a small thickness relative to its lateral extent) that has undergone brittle and/or ductile deformation. The commonly used term “fracture zone” can be used to denote a brittle deformation zone, or the brittle part of a composite deformation zone (a zone that shows evidence of both brittle and ductile deformation).

Lineament (Sw: lineament): A linear anomaly on the Earth’s surface, straight or gently curved, which has been interpreted based on a 2D data set. A lineament can, but does not necessarily, indicate a geological structure (e.g. a deformation zone or a rock dyke).

Unit (Sw: enhet): A unit is the smallest, undivided volume in a 3D geological model. Depending on its properties and intended use, the following qualifiers may be applied: rock unit (lithological unit) and structural unit (e.g. within a deformation zone) in bedrock models, and, for example, soil units in models that include superficial deposits.

Domain (Sw: domän): Units, for example rock units, can often be grouped together into domains with reference to a particular property. Thus, a geological domain in the bedrock can consist of several rock units with similar characteristics in terms of a particular property. Units with similar hydraulic properties can be grouped into a hydraulic domain, irrespective of differences in other properties.

Definitions related to the description of fractures and fracture zones in geological models are given in Section 3.2. Other terminology with relevance for transport properties modelling is given in Section 2.10.

1.4 Models produced at different stages of the site investigations

As described in the general programme /SKB, 2001b/, the Site Investigations are carried out in different stages, in which different versions of the Site Descriptive Models will be presented. Table 1-1 summarises the investigation stages and the models produced. In particular, “Preliminary Site Description” is presented at the end of the Initial Site Investigation stage and “Site Description” after the Complete Site Investigation stage.

The phase prior to the Site Investigations was completed in 2002. SKB has presented a summary of the Feasibility studies /SKB, 2001c/, and a series of reports that describe the available data. The general models (Version 0) of the two sites, Forsmark and Simpevarp, where Site Investigations are carried out, have also been published (Forsmark – /SKB, 2002a/; Simpevarp – /SKB, 2002b/). As indicated in Table 1-1, these models are based on compilations of existing data. They provide important inputs to the Site Investigations, especially with regard to planning of field investigations and identification of relevant model areas.

Recently, a special project was conducted where data available from the Laxemar area, which is part of the Simpevarp site, was evaluated and interpreted into a Site Descriptive Model /Andersson et al, 2002/. The project was primarily a methodology test. A Site Descriptive Model in local scale was developed, corresponding to the models to be produced after the Initial Site Investigation (Version 1.2). However, the model did not include descriptions of surface ecosystems or transport properties.

Table 1-1. Different versions of the Site Descriptive Models to be produced during the Site Investigations /SKB, 2001b/.

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

1.5 Structure of the present report

Following the general introduction to site descriptive modelling in the present chapter, the descriptive transport modelling is presented in Chapter 2. The aim with Chapter 2 is to provide an overview of all the components of the transport properties modelling process and how the work will be performed, including objectives and scope, working procedure, input and output data, and interactions with other disciplines. The description in Chapter 2 is intended to provide all the necessary information for readers looking for a description of the whole process, without all the details of the different steps.

Chapter 3 summarises the site descriptive modelling within Geology, Hydrogeology and Hydrogeochemistry, which all provide important input data and models for the transport modelling. In Chapter 4, a more detailed background to the transport modelling is given, including descriptions of conceptual and mathematical models, output parameters, and modelling tools. The different steps in the site descriptive transport modelling process (cf. Figure 1-2) are described in Chapters 5–7; Chapter 5 describes the acquisition of transport data (Primary Data) through laboratory and in situ measurements, Chapter 6 the Primary Data evaluation, and Chapter 7 the three-dimensional modelling. Finally, interactions with other disciplines and integrated modelling activities are described in Chapter 8.

2 Site descriptive transport modelling

2.1 Objectives and scope

This report presents guidelines for developing Transport Properties Site Descriptive Models during the different phases of the SKB Site Investigation Programme (see Table 1-1). These Site Descriptive Models may be regarded as final products of the discipline-specific programme "Transport properties of the rock" /SKB, 2001b/. This programme includes field and laboratory measurements, which are a responsibility of the site characterisation organisations, and modelling of transport properties. The guidelines presented herein are intended to guide the practical implementation of interpreting site-specific data into Site Descriptive Models.

In this report, the word "transport" means transport of solutes (radionuclides and other dissolved substances) in the groundwater. The main objective of the discipline-specific programme "Transport properties of the rock" is to provide transport parameters for radionuclide transport calculations within Safety Assessment (SA). It is important to note that issues related to conservative assumptions and "safety margins", in terms of parameter values and/or processes considered, are to be handled primarily by SA, and not in the site descriptive modelling process.

The Site Description should include a complete description of the present situation in terms of the transport parameters required by SA, but SA may choose to consider other transport parameter values in the various scenarios they evaluate. This implies that the Transport Properties Site Descriptive Model also must include "basic" transport parameters in a format suitable for re-analyses and evaluation of alternative parameter values for SA. In addition, strategies and methods for such analyses are required. This is an important component of the guidelines presented in this document.

Transport parameters are also used in the development of Site Descriptive Models within other disciplines. Hydrogeology uses transport parameters in groundwater flow simulations where density dependence is considered (salt transport). Furthermore, transport of dissolved species is studied within the Hydrogeochemistry programme. The development of Transport Properties Site Descriptive Models is a part of the integrated evaluation and interpretation of the geoscientific conditions at the investigated sites. This process, which is described by /Andersson, 2003/, implies interactions between the different disciplines, with the aim to achieve a consistent description of the geoscientific understanding of the sites.

In summary, the objectives of the site descriptive modelling process and the resulting Transport Properties Site Descriptive Models are to:

- Provide transport parameters for SA. Each model will include a set of parameters that describe the present situation, including the uncertainties in the parameters, as well as a basis for development of alternative parametrisations.
- Describe the geoscientific basis for the transport model, that is, the qualitative and quantitative data that are of importance for the assessment of uncertainties and confidence in the transport description, and their implications.

- Provide transport parameters for use within other discipline-specific programmes, e.g. Hydrogeology and Hydrogeochemistry.
- Contribute to the integrated evaluation of the investigated sites, including the assessment and presentation of the overall confidence in the models presented and the geoscientific understanding of the sites.

For example, data produced within the Transport programme can be used as a basis for calibration of hydrogeological models, whereas interactions between Geology, Hydrogeology and Transport are important for the allocation of parameter values to the geometric units described in the Site Descriptive Models. In addition, the identification of rock volumes or structures characterised by unfavourable transport properties is important information for Design /SKB, 2002b/.

In view of the identified objectives of site descriptive transport modelling and the resulting models, and the associated needs for methodological co-ordination, the objectives of this report are to:

- Present a description that gives an overview of the strategy for developing Site Descriptive Models, and which sets the transport modelling into this general context.
- Provide a structure for developing Transport Properties Site Descriptive Models that facilitates efficient modelling and comparisons between different sites.
- Provide guidelines on specific modelling issues where methodological consistency is judged to be of special importance, or where there is no general consensus on the modelling approach.

It is emphasised that the guidelines for site descriptive transport modelling, as described in the present document, do not form a strict and detailed instruction for how to carry out this complex task. The main intent is to present guidelines that provide some basic structure and guidance to the modelling process. It is also understood that further development of the guidelines may be needed. This need for further development may be more pronounced for Transport than for the other disciplines, partly because Transport was not included in the previous methodology test /Andersson et al, 2002/. Furthermore, transport modelling is the focus of several ongoing research projects, which likely will have impact on the site descriptive modelling when completed.

Finally, it should be noted that the present document is focused on the description of solute transport in the fractured rock outside a repository. This implies that parameters and models for source term modelling and for solute transport in the regolith (unconsolidated deposits) are not included in this report.

2.2 Overview of processes and parameters

2.2.1 Processes and parameter categories

Figure 2-1 shows a schematic illustration of the processes influencing solute transport in fractured rock. Essentially, solutes are transported by the flowing groundwater, by advection, under the influence of various processes that act to retard, immobilise, and/or transform the solutes /SKB, 2001b/. The conceptualisation of transport is based on a subdivision of the medium into mobile and immobile zones, where the distinction is made with regard to the presence of flow and advective transport. Specifically, the fractures and fracture zones where groundwater flow takes place are mobile zones, whereas the rock mass between the water-conducting features and various geologic materials within and in the immediate vicinity of these features are immobile zones. This is sometimes also referred to as a dual-porosity concept.

Given this general conceptualisation of solute transport, the main components of the transport description are the advection process in the mobile zones, the mass transfer between mobile and immobile zones, and the processes that act to transport, immobilise and transform the solutes within the immobile zones. Radionuclides are affected by radioactive decay in both mobile and immobile zones. Since this process is parametrised separately, based on generic data, it is not discussed further here. Thus, the processes that need to be described, qualitatively and quantitatively, based on site-specific information, can be separated into advection (including dispersion and channelling effects) and retention processes, where retention refers to all processes that retard, immobilise or transform the migrating solutes.

In models of radionuclide transport in fractured rock, the main retention processes are usually considered to be diffusion and sorption. In particular, diffusion and sorption within the rock mass ("matrix diffusion" and sorption on the inner surfaces of the rock) are in most cases identified as the most important retention processes in the long-term perspective of performance assessment calculations. However, also other processes, primarily hydrogeochemical processes such as precipitation, and other geological materials, e.g. fracture-filling materials, may be important for retention and solute transport. Thus, hydrogeochemical information and a detailed geological characterisation are important for the development of site-specific understanding of retention processes.

Concepts, processes and mathematical models related to site descriptive transport modelling are presented in Chapter 4. In short, the modelling approach for radionuclide transport is based on a quantification of transport parameters along flow paths. The description of these flow paths, that is, their locations within the 3D geometric model and the parameters that quantify solute transport along them, are obtained by particle tracking simulations in groundwater flow models. Specifically, "effective" parameters that describe advection and retention are quantified by integration of flow and retention parameters along flow paths between source (e.g. canister positions within a repository layout) and exit locations (e.g. a discharge area). Thus, the following parameter categories are described within the site descriptive transport modelling:

- *Parameters that characterise the retention properties of geologic materials*. This part of the description consists of parameters that quantify the diffusion and sorption properties of intact (fresh) and altered rock, fracture coatings and fracture-filling materials. These parameters are described within the framework of the 3D geometric models that are devised primarily by Geology.

- *Parameters that characterise solute transport along flow paths, here referred to as flow-related transport parameters.* These parameters are obtained by means of particle tracking simulations in groundwater flow models. They cannot be fully described within the 3D geometric modelling framework. Rather, the main geometric reference for these parameters is given by the starting positions of the paths.

The above parameter categories provide a basis for radionuclide transport calculations within SA. However, transport parameters are required also for modelling within some of the other disciplines, and for the integrated evaluation that aims to develop the general geoscientific understanding of the site. In particular, it is foreseen that Hydrogeology and Hydrogeochemistry, will perform calculations that require input from Transport. Differences in modelling approaches and model scales may imply that other parameter values, or even other parameters, than for radionuclide transport are needed in these simulations.

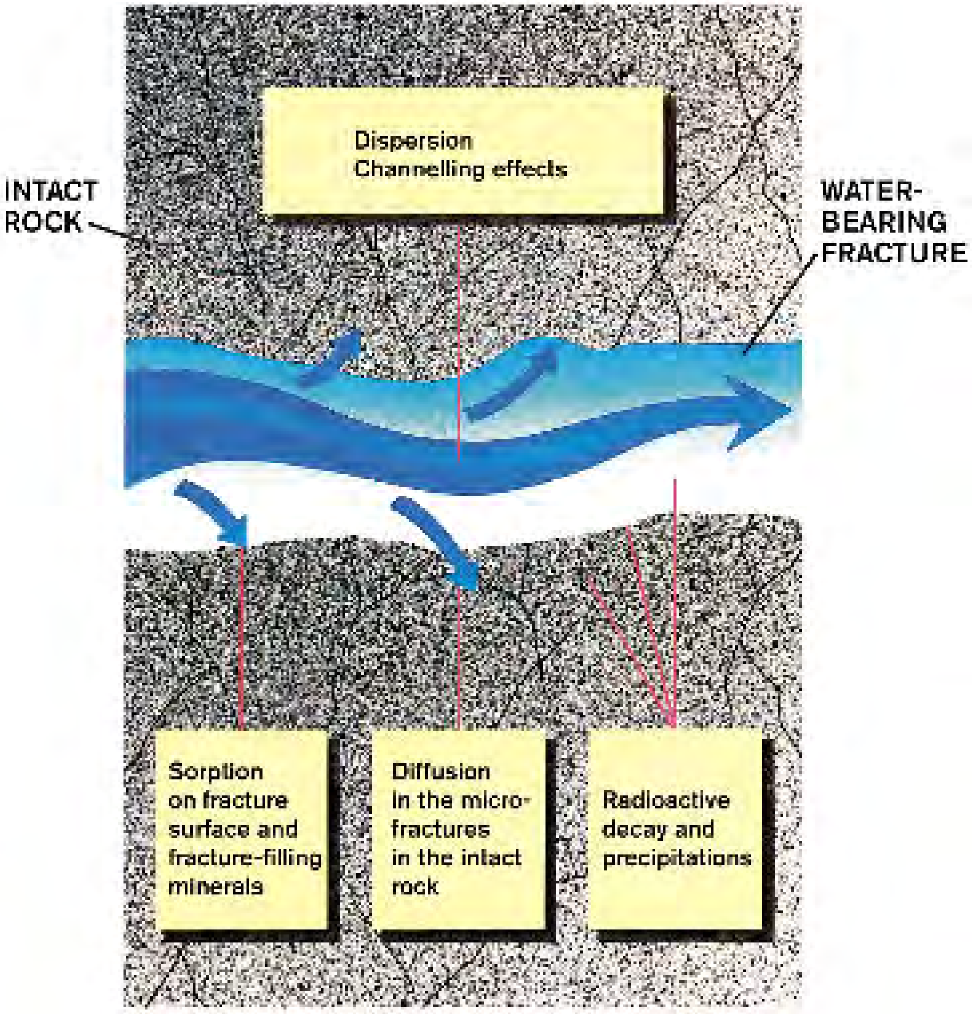


Figure 2-1. *Illustration of a flow path and the basic transport processes.*

2.2.2 On the basis for the present strategy

As explained in more detail below, the strategy for site descriptive transport modelling consists of a strategy for laboratory measurements and interpretations of the results (presented by /Widestrand et al, 2003/), and a strategy for site descriptive modelling (this report). Both the laboratory strategy and the modelling strategy have been developed primarily on the basis of experiences and models from previous SKB research and safety assessment projects.

In particular, laboratory methods and conceptual and mathematical models in the strategy documents are to large extent derived from the TRUE (Tracer Retention Understanding Experiments) programme /Byegård et al, 1998; Winberg et al, 2000; Andersson et al, 2002c/ and research within the framework of Äspö Task Force, whereas the identification of processes and parameters for SA calculations is based on the analyses performed in connection with the SR 97 project /SKB, 1999a/. These main inputs to the present work should be noted, especially since the strategy documents are not intended to contain complete background or state-of-the-art descriptions of the various modelling disciplines.

2.2.3 Retention modelling approach

Matrix diffusion and sorption are the main retention processes to be quantified within the site descriptive transport modelling. Specifically, sorption is modelled as a linear equilibrium process, that is, by a K_d-based approach. Since there are alternative approaches, both to the implementation of a K_d-based approach and to the modelling of retention in general, we present here the main features of the proposed modelling strategy for retention, leaving the details for Chapters 4 and 7:

1. Primary Data on site-specific diffusion and sorption parameters are obtained primarily from laboratory measurements on samples of rock cores.
2. Laboratory sorption measurements (batch sorption tests) are performed using different water compositions identified as typical for the site, thereby providing an empirical basis for quantifying the dependence of sorption on hydrogeochemistry.
3. In situ measurements will be used mainly for investigating spatial variability in retention properties, provided on-going methodology tests are successful.
4. Diffusion and sorption parameters are interpreted and assigned to typical, site-specific geological materials according to a strategy that combines site-specific transport data and input from other disciplines with expert judgement.
5. Geological and hydrogeochemical data and models are used to evaluate uncertainties and to assess site understanding and model confidence. In this assessment, qualitative evidence for the proposed retention mechanisms is analysed and described, but it could also include alternative process quantifications.
6. Particle-tracking simulations in groundwater flow models developed by Hydrogeology are used to investigate and account for spatial variability in retention along flow paths. The flow models are based on the geological and hydrogeological models of the sites, thereby accounting for all underlying site-specific data on fractures, fracture zones, and their properties.

Referring to the last point above, it should be noted that there is a distinction between different types of transport modelling. Site descriptive transport modelling refers to the process of assigning parameter values to geometric elements and flow paths. Transport modelling, as the notion is usually understood, implies that some sort of mathematical model is used to calculate, e.g. travel times, concentrations or mass fluxes. In the present context, mathematical modelling is one of the tools that will be applied in the site descriptive transport modelling.

2.3 Components of the site descriptive transport model

As described in more detail in Chapter 4, the transport models that will be produced during the Site Investigations include the following transport parameters for radionuclides:

- Diffusion and sorption parameters for geologic materials associated with rock units and structures ("matrix" parameters):
    - effective diffusivity, D_e [L^2T^{-1}],
    - sorption distribution coefficient, K_d [L^3M^{-1}],
    - porosity, θ_m [–],

  These parameters are described in Section 4.6.1 (see Table 4-2).
- Flow-related parameters for flow paths calculated for the present groundwater flow conditions:
    - water travel time, t_w [T],
    - "F-parameter", F [TL^{-1}].

  These parameters are described in Section 4.6.2 (see Table 4-3). Additional flow-related parameters, primarily "effective retention parameters" for flow paths, will be presented in models that involve spatially variable diffusion and sorption parameters.

In addition to numerical values of primary parameters (and quantifications of uncertainties), the Site Descriptive Models should also include quantitative and qualitative data and descriptions that can be used to assess the confidence in the model and the understanding of the site. For the transport properties model, this implies that data supporting the processes included in the model, and/or complementary descriptions of retention, should be presented.

The site descriptive transport modelling also involves interactions regarding parameters for transport modelling within other disciplines:

- Transport parameters for calculations of salt transport in groundwater flow models: dispersivities, "effective" flow and transport porosities, mass transfer parameters (different parameters are used in different flow models).
- Transport parameters for coupled hydrogeochemical and transport modelling: dispersivities and "effective" porosity, or travel time distribution (depending on modelling approach).

These modelling activities, and the associated parameters and interactions, are discussed in Section 4.7. At present, however, deliverables/parameters have not been specified.

Flow-related transport parameters will be calculated both within the site descriptive transport modelling and by Safety Assessment. The distinctions between these two modelling activities can be described as follows:

- The main objective of the calculations of flow-related parameters within the site descriptive modelling is to analyse the effects of spatial variability in diffusion and sorption parameters along flow paths. Thus, the calculations are used to address the issue of upscaling sorption and diffusion parameters by integrations along flow paths.
- The site descriptive modelling presents flow-related transport parameters for the present conditions regarding, primarily, hydrogeological and hydrogeochemical conditions. The aim is to contribute to the geoscientific understanding of the investigated sites by providing quantitative information on differences in transport conditions within the model volumes. Thus, release locations of particles are selected such that the whole model volume of interest is covered.
- SA calculates flow-related parameters for scenarios that consider future conditions and releases of radionuclides from the planned repositories. It follows that the calculations performed by SA may involve other flow and transport conditions, due to, for instance, changes in the flow pattern, and release locations determined by repository layouts. SA may also investigate other more specific issues related to the transport parameters, if such issues are identified as important for the safety evaluations.

The modelling strategy and the data deliveries described in this report (Chapters 5–7) concern the site descriptive modelling. However, the theoretical background (Chapter 4) and the methods for calculating flow-related parameters (Chapters 4 and 7) are valid also for the transport modelling within SA.

2.4 Working methodology

2.4.1 Overview and presentation of the guidelines

Figure 2-2, modified from the general execution programme /SKB, 2001b/, gives an overview of the development of Transport Properties Site Descriptive Models in the different phases of the Site Investigation. Generally, the site descriptive modelling is dependent on a relatively large quantity of site-specific data and of the work performed within other disciplines for meaningful modelling to be possible. The contributions from other disciplines are described in Section 2.6.

Many of the field and laboratory methods that are employed to obtain site-specific values of transport parameters are relatively time-consuming. Due to the limited availability of site-specific transport data in the early stages of the Site Investigation, the uncertainties associated with the parametrisation of the 3D geometric model will be relatively large in the model versions presented during the Initial Site Investigation. At this stage, the transport programme is focused on commencing time-consuming laboratory measurements and on identifying unfavourable transport conditions, primarily using data and models produced within other disciplines /SKB, 2001b/. As indicated in Figure 2-2, comparisons with generic (non site-specific) data will be made during the Initial Site Investigation. The compilation of a generic transport database may be viewed as the equivalent of the Version 0 modelling work that previously has been carried out within other disciplines.

The transport properties modelling during the Complete Site Investigation will to a much larger extent be based on site-specific transport data. However, the inputs from other disciplines are important also at this stage. As mentioned above, flow-related transport parameters are to be calculated using hydrogeological models. Furthermore, Geology and Hydrogeochemistry provide important inputs for the selection and analyses of rock samples, and for the parametrisation of geological units with retention parameters. During the Complete Site Investigation, the work with laboratory and field measurements and transport modelling will be performed as an iterative process.

The guidelines for Transport Properties Site Descriptive Modelling are presented in the current document and in the report “Strategy for the use of laboratory methods in the site investigations programme for the transport properties of the rock” /Widestrand et al, 2003/. Whereas the current document describes the whole process of site descriptive modelling, /Widestrand et al, 2003/ focus on the collection, analysis and interpretation of diffusion and sorption data. The result of the work described in their report will be delivered as an input to the transport modelling in the form of a “retardation model”. The relation between the two documents that present the transport modelling guidelines is indicated in Figure 2-2. It can be seen that both reports cover modelling aspects; the contents of the “Laboratory strategy report” are summarised in Chapters 5 and 6 of the present report.

The different amounts of site-specific data available during the early (Initial) and late (Complete) stages of the Site Investigation are reflected in the aims/ambitions associated with different model versions /SKB, 2001b/. As a consequence, much of what is said below about parametrisation of geological elements and calculation of flow-related transport parameters, especially the “averaging” of retention properties along flow paths, is applicable to the modelling work during the Complete Site Investigation only. In the following, specific guidelines for the models to be produced during the Initial Site Investigation will be presented as needed. Given the overall time-plan of the Site Investigations, and the fact that important transport-related research is still in progress (primarily at Äspö HRL), further developments of the guidelines for modelling during the CSI stage are likely.

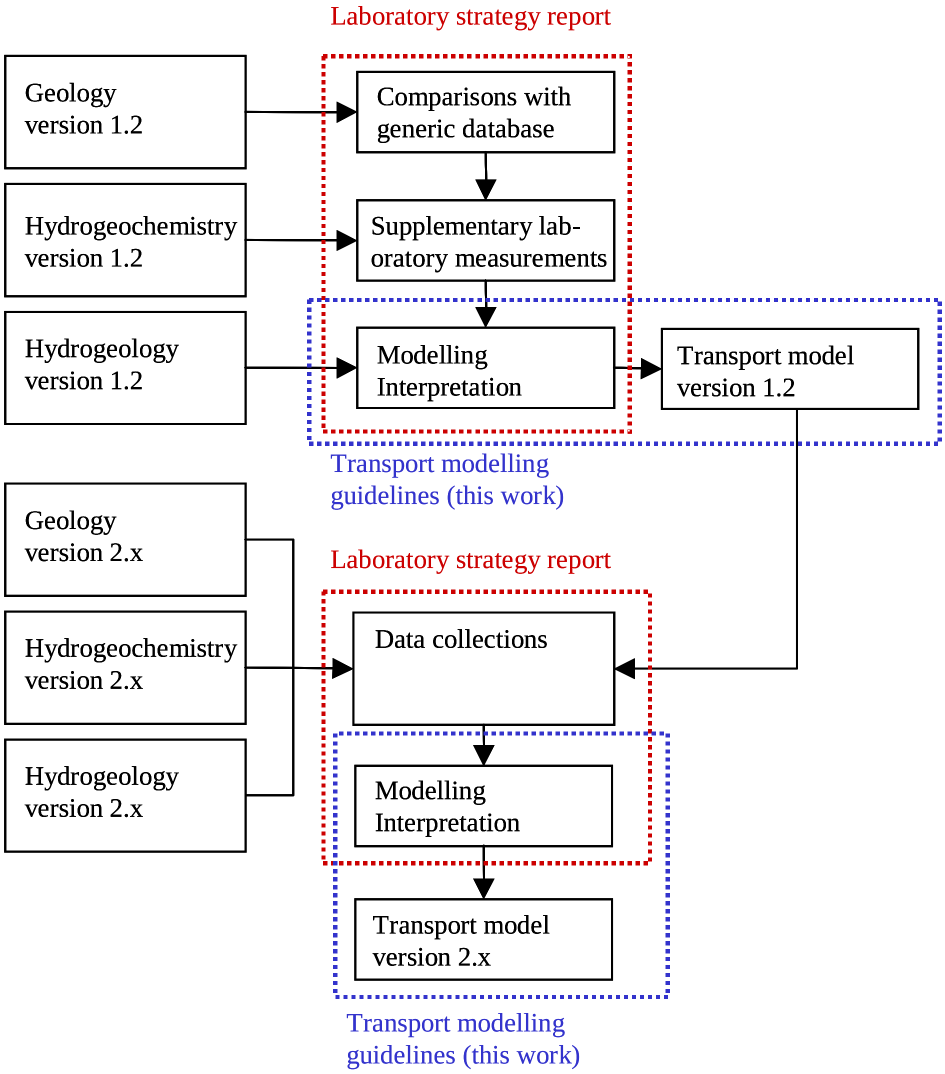


Figure 2-2. *Working methodology for development of Transport Properties Site Descriptive Models /from SKB, 2001b/. The relation between the current document and the "Laboratory strategy report" /Widestrand et al, 2003/ is indicated.*

2.4.2 Description of the modelling procedure

The general procedure for site descriptive modelling, applicable to any model version, is presented in Section 1.2.2. An overview of the modelling procedure for developing transport properties models is illustrated in Figure 2-3. Note that the flow chart is intended to describe the development of a single, "generic" model version, and that it is highly simplified, especially with respect to interactions with other disciplines and feedbacks from assessment steps. More detailed descriptions of the various activities and model components involved in the modelling procedure are provided in Chapters 5 through 7.

The modelling procedure consists of the following basic parts:

1. Identification, acquisition and control of input data:

- Identification of relevant generic (non site-specific) data.

- Interactions with Investigations in the process of sample selection, planning of in situ measurements, analyses of data from in situ and laboratory measurements, and database development, in order to ensure timely access to site-specific transport data.
- Interactions with other disciplines, primarily Geology, Hydrogeology and Hydrogeochemistry, in order to access relevant data and models.

2. Evaluation of primary data:

- Interpretation of diffusion and sorption parameters and development of retardation model.
- Evaluation of in situ measurements (e.g. tracer tests).

3. Three-dimensional modelling:

- Parametrisation of geologic elements (deterministic structures, stochastic fractures, and intact rock) with retention parameters.
- Integration along flow paths in hydrogeological models to obtain flow-related transport parameters (effective advection and retention parameters for flow paths).
- Assessment of confidence and uncertainty, including evidence for proposed retention processes and alternative/complementary process quantifications.

4. Overall confidence assessment:

- Consistency among modelling disciplines.
- Comparison between new and previous models.
- Discussion on the value/effects of additional measurements.

5. Documentation and data deliveries:

- Documentation in databases (primarily SICADA), RVS, and reports.
- Data deliveries to Safety Assessment, Design, and other modelling disciplines.

Essentially, Stage 1 results in a site-specific database with retardation parameters (see definition in Section 2.10), and Stage 2 in a “retardation model” that consists of parameterised “typical” rock units and “type structures”. In the three-dimensional modelling (Stage 3), the retardation model is used to assign (groups of) parameter values to geological units in the geometric site model. Also, flow-related transport parameters are calculated by integration in groundwater flow models, using the three-dimensional description of retardation parameters as additional (non-hydrogeological) input when quantifying spatially variable retardation parameters.

The three-dimensional transport properties modelling should be regarded as an integrated activity, where the results of the retardation parameterisation can be used in the quantification of flow-related parameters. However, the level of integration will increase as the Site Investigation proceeds. In the models produced during the Initial Site Investigation, the descriptions of retardation and flow-related parameters are developed and reported more or less separately, whereas the modelling during the Complete Site Investigation aims at a “fully integrated” retardation parameterisation in the groundwater flow models. This is indicated by the dashed connectors in Figure 2-3; retardation parameters may either be transferred to the flow models (that is, be included in the flow models by a parameterisation of the elements in the models), or be handled separately. In the latter case, only hydrodynamic parameters are calculated in the flow models.

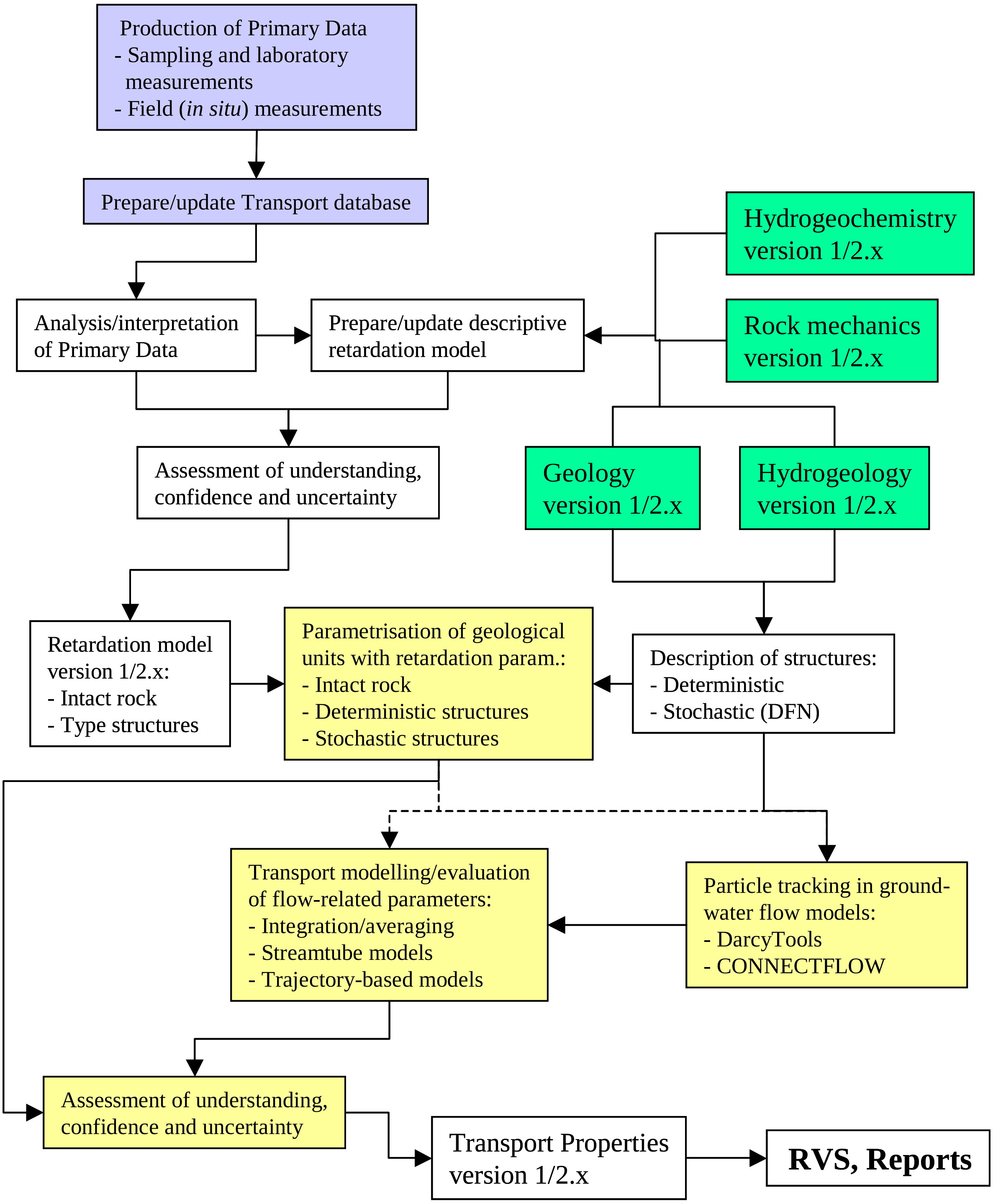


Figure 2-3. *Working methodology for the development of Transport Properties Site Descriptive Models. The geometric framework for the Site Descriptive Model is provided by the RVS (Rock Visualisation System) model that describes the geological units at the site. Yellow boxes indicate the main modelling activities described in this report, whereas blue and green boxes are activities that produce transport-specific input data and descriptions provided by other disciplines, respectively.*

Stage 4 is an integrated activity involving all disciplines. Consistency checks among the different disciplines are important components in the evaluation of the overall confidence in the description. Furthermore, it is important to assess the potential value of additional measurements for increasing the confidence and reducing the uncertainties associated with the description. Note that even though "Documentation and data deliveries" is listed as the final step, "Stage 5" above, these activities will be carried out continuously during the modelling process, as needed by the users.

Stages 1 and 2 are described in detail by /Widestrand et al, 2003/, with particular focus on laboratory measurements of diffusion and sorption properties. Suggested procedures and modelling-related guidelines for data acquisition and evaluation are summarised in Chapters 5 and 6, respectively, of the present document. The three-dimensional modelling is described in Chapter 7. Finally, Chapter 8 contains guidelines related to data deliveries and other interactions, primarily with the other modelling disciplines.

2.5 Transport data

Transport parameters were not included in the data compilation work that was performed in connection with the Feasibility Studies, and transport properties modelling was not considered in the Site Descriptive Models Version 0 of the two sites where Site Investigations are being carried out. Hence, no transport data is available from these previous data compilations and models. However, transport parameters and models have been studied by SKB and others in a number of research projects during the last 25 years /e.g. Byegård et al, 1998; Winberg et al, 2000; Andersson et al, 2002c/. As a result of this work, a relatively large amount of generic data is available that can be used for preliminary modelling and comparisons with the data gathered during the Site Investigations.

Data on sorption and diffusion parameters were compiled during the SR 97 project. Specifically, /Carbol and Engkvist, 1997/ compiled and presented available sorption data, whereas /Ohlsson and Neretnieks, 1997/ presented a compilation of diffusion data, see also the SR 97 "Data report" /Andersson, 1999/. These databases will be updated during the Site Investigations. Since the Site Investigations are carried out in areas where some of the previous transport investigations were performed, we may distinguish between two types of "generic" data:

- *Data obtained from investigations in the vicinity of, or even within, the prioritised Site Investigation areas.* This type of data could provide information on the retention properties of materials in the geological units at the Sites. There may, however, be some discrepancies between the Site Investigations and previous studies in terms of the methods used for sampling and analyses, and the hydrochemical conditions in the experiments.
- *Data from other sites, in Sweden and elsewhere.* This type of data may serve as general references and be useful for establishing parameter intervals for wider classes of geological materials. As compared to Site Investigation data, differences can be expected regarding both the geological conditions and the investigation methods used.

Common to both categories of generic data is that their usefulness for site descriptive modelling should be evaluated based on the geological properties, the methods used to obtain the data, and the hydrochemical conditions. Obviously, this requires that the geological properties of the samples underlying the databases are known. In some cases, that is, when the samples are still available, it may be motivated to "upgrade" the generic data by complementary geological characterisation.

During the Site Investigations, site-specific transport data will be collected by in situ and laboratory measurements. Whereas generic data are important in the early stages (during the Initial Site Investigation), when only limited site data is expected to be available, the site descriptive models developed during the Complete Site Investigation will mainly rely on Site Investigation data. The characterisation methods employed within the Transport programme, and the associated Method Descriptions (MD), are summarised in Table 2-1.

The laboratory methods, except for gas diffusion measurements, can be regarded as relatively well established, whereas most of the field/in-situ methods are still under development. Some of the field methods will be tested during the Initial Site Investigation. In addition, transport modelling may also be regarded as a "characterisation method". Specifically, transport modelling will be used to quantify transport parameters for Safety Assessment, and to contribute to the joint interpretation of site conditions and the development of a geoscientific understanding of the site.

Table 2-1. Summary of investigation methods, parameters, and Method Descriptions within the Transport programme.

Method	Parameters	MD # / comment
Laboratory measurements		
Through diffusion (in aqueous phase) measurements	Diffusivity Porosity Sorption coefficients	MD 540.001
Laboratory electrical conductivity (resistivity) measurements	Diffusivity	MD 230.001 (Geology)
Gas diffusion measurements	Diffusivity Porosity	Limited use – no MD required
PMMA porosity measurements	Porosity	MD 540.003
Water saturation porosity measurements	Porosity	Described in MD 540.001
Batch sorption measurements	Sorption coefficients	MD 540.002
Field measurements		
In-situ electrical resistivity measurements (logging)	Diffusivity	To be tested during ISI – possibly MD later
Groundwater flow measurements	Flow rate, velocity	MD 350.001
Single-well injection-withdrawal tests (SWIW)	Advection and retention parameters*	To be tested during ISI – possibly MD later
In-situ tracer sorption/diffusion (single-hole tracer, in-situ retention)	Diffusivity Sorption coefficients	Theoretical study incl. scoping calculations under way
Multi-well tracer tests	Advection and retention parameters*	MD 530.006
Radon measurements	Flow-wetted surface	To be further evaluated

* Depends on experimental setup (e.g. tracers used) and evaluation model.

2.6 Inputs from other disciplines

The Transport Properties Site Descriptive Modelling depends to a relatively large extent on data and models produced within other disciplines. The most important interactions that provide inputs to the site descriptive transport modelling are summarised in Table 2-2.

As indicated in Table 2-2, the inputs received from other disciplines include specific parameters as well as contributions to integrated analyses. In particular, the parametrisation of geological units with retardation parameters requires a close co-operation with Geology, Hydrogeology and Hydrogeochemistry. Concepts and parameters used within these disciplines are further discussed in Chapter 3.

Table 2-2. Inputs from other disciplines.

Discipline	Interaction/input to transport modelling
Geology	Geometry of deterministic structures
	Description of stochastic fractures (Discrete Fracture Network, DFN)
	Rock type distribution
	Porosity data
	Integrated analyses for parametrisation of intact rock, fractures and fracture zones with retardation parameters
Hydrogeology	Flow distribution, flow paths for calculation of flow-related transport parameters
	Hydraulic properties of deterministic structures
	Description of conductive stochastic fractures, incl. hydraulic properties (DFN)
	Integrated analyses for parametrisation of intact rock, fractures and fracture zones with retardation parameters
Hydrogeochemistry	Groundwater chemistry, processes affecting the water composition, typical water compositions (input data for sample selection and laboratory measurements)
	Fracture mineralogy and hydrochemical parameters and models for assessment of site understanding and model confidence (evidence of processes and basis for alternative/complementary conceptual and mathematical retention models
Rock mechanics	Stress state (supporting data for interpretation of laboratory data)

2.7 Output data and contributions to other disciplines

The methods summarised in Table 2-1 generate mainly parameters that describe the diffusion and sorption properties of the sampled geological materials. These parameters are to be further evaluated and associated with the geological units at the site, that is, be presented in a Site Descriptive Model. Presented in this format, the parameters are accessible for further analyses within the transport programme and by others (e.g. Safety Assessment).

Flow-related transport parameters, including integrated retardation parameters, will be calculated based on modelled flow distributions that represent the present situation. Other scenarios may be developed and modelled within the framework of Safety Assessment. The flow-related parameters, which are not described within the geometric framework of the geological units (the geometry of a flow path, and the information included in its associated flow-related parameters, are determined by the flow field), are presented in reports.

Table 2-2 lists various interactions between Transport and other disciplines, with emphasis on the inputs to transport modelling from others. However, some of the methods and modelling activities within the Transport programme will also contribute to the Site Descriptive Modelling within other disciplines. In the integrated analyses for parametrisation of fractures and fracture zones, transport data (and more qualitative observations) may provide supporting data for the geological and hydrogeological descriptions. Some of the in situ methods in Table 2-1, primarily groundwater flow measurements and multi-hole tracer tests, are (potentially) important for hydrogeological modelling and overall confidence assessment. Tracer tests and their role in the site descriptive modelling process are described in Chapter 8.

2.8 Model scales

Several temporal and spatial scales are relevant for the site descriptive transport modelling. The temporal scales are mainly related to the investigation methods employed, and their ability, or inability, to describe processes and parameters that are relevant for the end users. In particular, we may distinguish between a “Tracer test time scale” (a few months to a few years), which is relevant for the evaluation of tracer tests and for the description of early stages of radionuclide transport scenarios, and a “Safety Assessment time scale” (typically a few thousand or tens of thousands of years), e.g. /Dershowitz et al, 2003/. In addition, a “Resaturation time scale” is relevant for the description of the processes that take place after closure of the repository.

The assignment of “effective” retention parameters for different temporal scales or regimes is strongly linked to the spatial variability of the underlying parameters. Specifically, previous investigations at Äspö HRL /Byegård et al, 1998; Xu and Wörman, 1998/ have demonstrated that retention properties are spatially variable, both laterally and along fracture planes and in the direction perpendicular to the fracture planes (into the matrix). A gradient in the retention properties perpendicular to the fracture implies that different values of “effective” retention parameters at different times during solute penetration into the matrix /see Cvetkovic and Cheng, 2002/. Note, however, that not only the primary transport parameters (diffusion and sorption parameters) may be important for the effects of temporal variations. For example, long-term transients in groundwater flow and hydrogeochemistry may have to be addressed in the quantification of retention and flow-related transport parameters on the SA time scale.

All input parameters are spatially variable to some extent, and it is necessary to describe the spatial variability of the parameters in the Site Descriptive Models /Andersson, 2003/. A wide range of spatial scales needs to be considered in the transport properties modelling. The characteristic scales of spatial variability (correlation scales, etc) that can be associated with a certain parameter determine whether/on what scale the spatial variability in that parameter must be considered. The methods used to obtain parameter values determine the smallest scale that can be modelled (through the sample size), and the potential for characterising spatial variability at a given scale (through the number of samples).

The parameter values included in the Site Descriptive Models should be associated with the scale of the description. Site Descriptive Models are to be presented in Local and Regional scales. The spatial resolutions of these models determine the required resolutions of the parameters in the descriptions. Furthermore, the “Repository scale” is an additional spatial scale with particular relevance for developing an understanding of the transient phases during construction and after closure of the repository.

The scales considered in the hydrogeological models that are used to calculate flow-related transport parameters must be consistent with the scales of the modelled transport scenario. The relevant transport scales are determined by the “release scale” (e.g. individual canisters) and the “observation scale” (e.g. point sampling, or integrated observation in discharge areas). It should be noted that the scale of a description is to be decided by the user, not by the modeller, since it is determined by the requirements imposed by the subsequent analyses /Andersson, 2003/.

2.9 Management of uncertainties

In addition to the primary data produced within the transport investigation programme (Table 2-1), the transport properties modelling relies on data and models from other disciplines (Table 2-2). Consequently, the resulting Transport Properties Site Descriptive Model is subject to uncertainties related to measurements and interpretations of primary transport parameters, as well as uncertainties in, primarily, geological interpretations and hydrogeological and hydrogeochemical models. In particular, the flow-related transport parameters are obtained from hydrogeological models, which means that the uncertainties in these models are propagated to the transport description.

The strategy for management of uncertainties that will be implemented during the site descriptive modelling work is described by /Andersson, 2003/, who also defines some basic terminology. The different categories of uncertainties to be assessed, and (to some extent) quantified, during the Site Investigations are *conceptual uncertainty* and *data uncertainty*. Conceptual uncertainty concerns the uncertainty originating from an incomplete understanding of the structure of the analysed systems and its interacting processes. This uncertainty is comprised both of lack of understanding of individual processes and the extent and nature of the interactions between the processes. Such uncertainties can be identified for the description of retention in the transport modelling. For the Site Descriptive Model, incomplete understanding of the basic geometrical structures of the rock is also a conceptual uncertainty.

Data uncertainty concerns uncertainty in the values of the parameters of a model, that is, uncertainty about the properties. Such uncertainties may be caused by, for example, measurement errors, interpretation errors, or the uncertainties associated with extrapolations of parameters that vary in space, and possibly also in time. It should be noted that spatial variability is not uncertainty *per se,* because it can be well recognised and understood (it is a real and observable property of the system). However, spatial variability is often an important source to data uncertainty, because parameters that exhibit large spatial variations are difficult to evaluate beyond the local region of their measurement.

The Site Descriptive Models shall include quantifications of the data uncertainties in the parameter values. The representation of data uncertainty can be stochastic or deterministic, discrete or continuous. In addition, the origin of data uncertainty should be described /Andersson, 2003/. Uncertainties that cannot be described as data uncertainty distributions can be assessed by means of alternative models. Alternatives may include alternative geometrical frameworks (e.g. the geometry of deformation zones), and alternative descriptions (e.g. different models or parameter values). For the transport properties description, it is anticipated that the primary transport parameters are subject to data uncertainties, whereas conceptual uncertainties may originate from the description of retention as well as from the underlying geological, hydrogeological and hydrogeochemical descriptions.

2.10 Definitions

Since transport properties modelling involves different types of transport parameters, and models developed within other disciplines, a long list of definitions would be required to cover all the aspects of the modelling work. Instead, we provide here references where different types of definitions are presented:

- ***Geological parameters and modelling definitions:*** /Munier and Hermanson, 2001; Munier et al, 2003/, see also Section 1.3,
- ***Hydrogeological parameters and modelling definitions:*** /Rhén et al, 2003/,
- ***Definitions related to retention processes:*** /Widestrand et al, 2003/,
- ***Definitions related to uncertainty, scale, variability, and confidence assessment:*** /Andersson, 2003/.

For convenience, some of the definitions given by /Widestrand et al, 2003/ are repeated here:

- **Immobilisation:** processes by which solutes become irreversibly incorporated within immobile solid phases within the geosphere (over the time scales of relevance to performance assessment).
- **Matrix diffusion:** transfer of radionuclides by diffusion (a process resulting from random motion of molecules by which there is a net flow of matter from a region of high concentration to a region of low concentration) between flowing groundwater in fractures to stagnant water in rock matrix pores.
- **Retardation:** reversible processes (**sorption** and **matrix diffusion**) that delay the time taken for solutes to traverse the geosphere.
- **Retention:** the combined effect of **retardation** and **immobilisation** processes that leads to a decreased net flow rate of solutes through the geosphere.
- **Sorption:** a collective name for a set of processes by which solutes become attached by physical or chemical reactions to solid surfaces within the geosphere. The term is

taken to include processes that are reversible over the time scales of relevance to performance assessment.

- **Retardation model:** the retardation model is an interpreted description (including interpreted data) of retardation properties for the typical rock units and structures at a site (different types of rock, fractures and local minor and major fracture zones). It consists of a rock unit description, a description of the typical layers (including their thickness) for fractures and fracture zones, and a database with interpreted porosity, sorption and diffusion data for the different materials. The retardation model is the final product of the laboratory investigations of the transport properties of the rock.

According to these definitions, and under the assumptions described in Chapter 4, "retention" is a general term for all processes, other than advection and dispersion, that affect transported solutes, whereas the term "retardation" covers the processes that are parametrised within the Transport programme. Therefore, we use "retention" when discussing processes in general, and "retardation" in most of the specific descriptions of processes and parameters related to the site descriptive modelling.

2.11 References

The main references for developing the guidelines presented in the current document can be categorised and summarised as follows:

- General descriptions of the Site Investigations, investigation methods, and site descriptive modelling: /SKB, 2000, 2001b).
- Strategies for site descriptive modelling within other disciplines: see list in Section 1.2.2; the methodology for geometrical modelling with RVS (Rock Visualisation System) is also described by /Munier and Hermanson, 2001/.
- Methodology test for site descriptive modelling (Laxemar): /Andersson et al, 2002a/.
- Processes of importance for repository development and Safety Assessment: /SKB, 1999/.
- Parameters to be estimated during the Site Investigations: /Andersson et al, 1998b, 2000/.
- Compilation of data and assessment of data uncertainties: /Andersson, 1999/.
- Compilations/databases of matrix diffusion and sorption parameters: /Ohlsson and Neretnieks, 1997; Carbol and Engkvist, 1997/.
- Recently developed in situ methods planned to be used during the Site Investigations: In situ formation factor logging: /Löfgren and Neretnieks, 2002, 2003/, Single-Well Injection-Withdrawal tests (SWIW): /Nordqvist and Gustafsson, 2002; Gustafsson, 2002/.
- General reviews of conceptual and mathematical models of transport in a single fracture (including extensive reference lists): /Bodin et al, 2003a,b/.

- Geological/hydrogeological conceptual models for fractures and flow paths, hydraulic parametrisation of flow paths: /Bossart et al, 2001 ; Dershowitz et al, 2003/.
- Geological/transport conceptual models for fractures and flow paths, parametrisation of fractures/flow paths with retention parameters: /Andersson et al, 2002c ; Poteri et al, 2002; Dershowitz et al, 2003/.
- Conceptual models for transport processes and evaluation of transport parameters from tracer tests: /Winberg et al, 2000; Cvetkovic et al, 2000; Cvetkovic and Cheng, 2002; Poteri et al, 2002; Elert and Svensson, 2001; Neretnieks, 2002; Neretnieks and Moreno, 2003/.
- Calculation of flow-related transport parameters in groundwater flow models: /Andersson, 1998a; Dershowitz et al, 1999; Gylling et al, 1999; Widén and Walker, 1999; Tukiainen, 2002; Cheng et al, 2003; Cvetkovic et al, 2004/.
- Process-based retention models: /NEA, 2001; Bruno et al, 1995, 1998, 2001, 2002/.
- Safety Assessment transport codes: Source-term/near-field code COMP23: /Romero et al, 1999/, Far-field (geosphere) code FARF31: /Norman and Kjellbert, 1990; Lindgren et al, 2002/.

It is evident from the list above that site descriptive transport modelling involves aspects of a number of different disciplines and subject areas. Obviously, only a very limited selection of the relevant references for all these disciplines can be presented here. It should also be noted that additional relevant inputs to the site descriptive modelling strategy could be expected from ongoing research efforts. Some ongoing or recently completed SKB research projects that are relevant for site descriptive transport modelling are listed in Table 2-3.

Table 2-3. Recent/ongoing research projects with relevance for transport modelling.

Project	Scale, L (m)	Main activities/inputs to Transport modelling	References
TRUE-1	Detailed scale, L < 20 (interpreted single conductive feature)	- Geological and hydro-geological characterisation - Laboratory measurements of retention properties - Tracer tests - Conceptual modelling - Predictive and inverse transport modelling	/Winberg et al, 2000; Byegård et al, 1998; Cvetkovic et al, 2000; Elert and Svensson, 2001/
TRUE Block Scale	Block scale, 20 < L < 200	- Hydrogeological characterisation and development of hydro-structural model - Laboratory measurements - Tracer tests Conceptual, predictive and inverse modelling	/Andersson et al, 2002c,d; Poteri et al, 2002; Winberg et al, 2002; Cvetkovic and Cheng, 2002/
Fracture Characterisation and Classification (FCC)	Block scale, 20 < L < 200 Site scale, 200 < L < 2000	- Geological descriptions of conductive structures - Alternative interpretations of observed transport behaviour	/Mazurek et al, 1997; Bossart et al, 2001/
Performance Assessment Modelling using Site Characterisation data (PASC; Äspö Task Force, Task 6)	Block scale, 20 < L < 200	- Development of “semi-synthetic” hydro-structural and micro-structural models - Parametrisation with hydraulic and transport parameters	/Dershowitz et al, 2003/
Long Term Diffusion Experiment (LTDE)	Detailed scale, L < 1	- Laboratory measurements of retardation parameters - In situ measurements of diffusion and sorption on fracture surfaces and intact rock	/Byegård et al, 1999/

3 Related Site Descriptive Models

3.1 General

The geoscientific Site Descriptive Models of a site are divided into geometrical units based on differences in properties. These differences shall be significant in some respect for the use of the model. As pointed out in /SKB, 2000, 2001b/, the main users of the Site Descriptive Models are Design and Safety Assessment. The descriptive models shall also be of such detail and content that they give a sufficient geoscientific understanding of the site in terms of processes, geometric description, and uncertainties to provide an overall confidence that the models are adequate for their purposes.

The aim of the transport properties site descriptive modelling is to produce transport parameters for geometrical/geological units and for flow paths. As described in the preceding chapter, this involves data and models from several other disciplines, which implies that the concepts and models used within these disciplines must, to some extent, be described and understood. In the following, some basic concepts underlying the geological, hydrogeological, and hydrogeochemical modelling are presented. The strategies for site descriptive modelling within Geology, Hydrogeology and Hydrogeochemistry are described by /Munier et al, 2003; Rhén et al, 2003; Smellie et al, 2002/, respectively.

Since the transport description is partly developed with the aid of interpretations based on (qualitative and quantitative) correlations with the parameters in the geological and hydrogeological descriptions, these parameters are summarised below. Regarding the interactions with Hydrogeochemistry, it may be noted that the use of hydrogeochemical data and models in connection with sample selection and laboratory analyses is described by /Widestrand et al, 2003/. However, hydrogeochemical data and descriptions will be used also in the transport modelling. Therefore, the strategy for site descriptive hydrogeochemical modelling is summarised in Section 3.4.

3.2 Geological/geometric modelling

3.2.1 Geological objects

The structure geological model used by SKB /Andersson et al, 2000; SKB, 2001b/ consists of rock mass units and four different size classes of structures: regional fracture zones, local major fracture zones, local minor fracture zones, and fractures within the rock mass, see Table 3-1 and Figure 3-1. This structural model is the basis for developing site descriptive models during the Site Investigations. Specifically, the rock mass units and structures identified and described by Geology is the starting point for parametrisation within other disciplines. However, other subdivisions of the rock may be found more appropriate for the other descriptions. Although both simplifications and more complex models are possible, these alternative subdivisions are in most cases likely directed towards simplifications of the basic geological model (e.g. by merging of rock units).

Table 3-1. Classification and terminology for fractures and fracture zones, and ambition level for geometric description during site investigation /from Andersson et al, 2000/.

Name	Length	Width	Ambition for description
Regional fracture zones	> 10 km	> 100 m	Deterministic
Local major fracture zones	1 – 10 km	5 – 100 m	Deterministic (with uncertainties)
Local minor fracture zone	10 m – 1 km	0.1 – 5 m	Statistical (some deterministic)
Fractures	< 10 m	< 0.1 m	Statistical

Among the various rock units and structures described, the large *deformation zones* are of primary interest, because they may have an impact on several of the discipline-specific descriptions. Furthermore, information on these zones is essential for Safety Assessment and Design. The large deformation zones, that is, *Regional fracture zones* and *Local major fracture zones*, are therefore important geometrical units to be defined in space. This is indicated by the references to a "Deterministic" ambition level in Table 3-1.

The ambition of a deterministic description concerns primarily the geometrical description of the zones; other parameters, e.g. transport parameters, may very well be described statistically. Some *Minor fracture zones* will also be described deterministically in space (more as the investigations proceeds), but most of them are described statistically (as stochastic distributions). *Fractures* will be considered as stochastic distributions only.

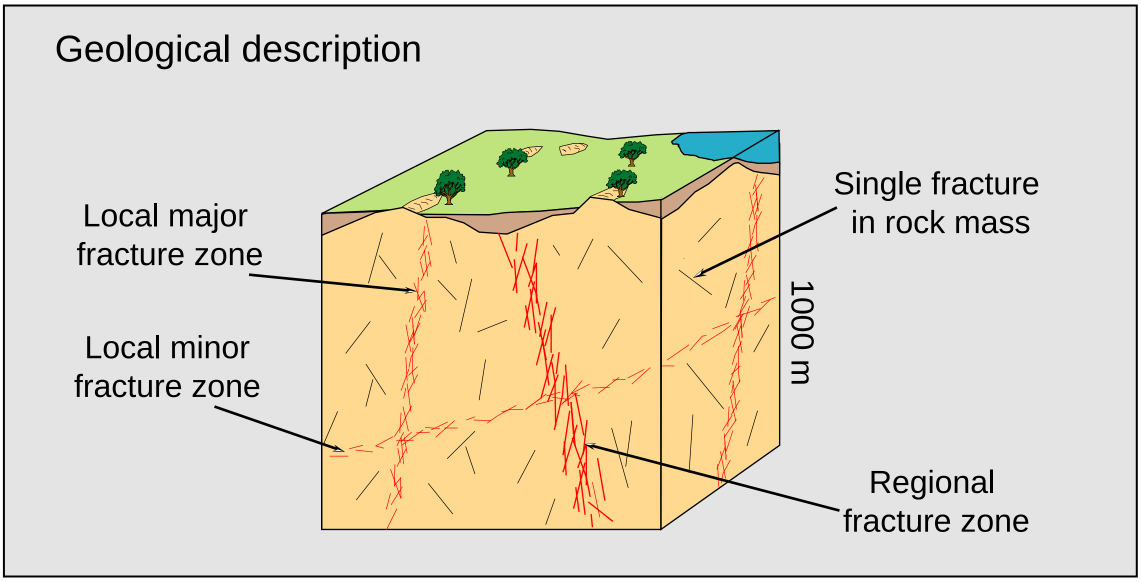


__Figure 3-1.__ Principal illustration of the main features of a geological model /from SKB, 2001b/.

Although the large zones are important also for the transport description, it should be noted that any realistic transport scenario involves a range of different structures. In the repository design, it is required that the deposition tunnels and deposition holes do not intersect, and have a respect distance to, regional and local major fracture zones /Andersson et al, 2000/. It is also required that deposition holes are not intersected by identified local minor fracture zones, and a low fracture density is preferred. The individual fractures within the rock mass are thus important, seen in a transport perspective, since they will likely act as the first water-conducting transport pathways in the rock barrier in a defect canister scenario. This implies that also the smaller structures must be described and parametrised with transport parameters.

3.2.2 Geological classification and parameters

Rock mass units and structures are identified and described in terms of a number of geological parameters /SKB, 2001b/. In order to give an overview of the geological information that will be available, these parameters are summarised in Table 3-2. The table is taken (in condensed form) from /Munier et al, 2003/; for a detailed description of the various parameters, we refer to their report. The identification of rock types and textural varieties of these units is an important input to the selection of samples for laboratory analyses of the diffusion and sorption properties of the rock mass within the Transport programme. Similarly, the sampling of structures is to large extent to be based on the results of geological investigations. The sampling-oriented interactions between Transport and Geology are further described by /Widestrand et al, 2003/.

The transport modelling is also closely related to the modelling work within Geology. In addition to the structural model itself, the geological parameters of importance for transport include, for example, the porosity, density, and fracture properties (densities, orientations, apertures (interpreted from visual observations), trace lengths, etc) of the rock mass, and the width and fracture properties of identified (deterministic) fracture zones. In particular, a DFN (Discrete Fracture Network) description of the stochastic fractures is provided by Geology. These parameters affect the transport modelling both directly in the process of assigning retention parameters to rock mass and structures, and indirectly through the joint geological/hydrogeological interpretations and the resulting hydrogeological models.

Table 3-2. Parameters in the geological description /from Munier et al, 2003; Table 5-2/.

Parameter	**Comment**
Rock properties	
Rocktype	Represents the *dominant* rock type
Grainsize	
Structure	
Fabric: Type	
Fabric: Orientation	Defined as constants or distributions
Porosity	All numeric properties (cf. below) can be given as a constant, a range (min-max) or a distribution
Susceptibility	Numeric
Density	Numeric
Gamma	Numeric
Alteration	Classification in terms of *fresh* and different degrees of *weathering*
Parameter	**Comment**
Fold axial plane	
Fold axis	
Mineral composition	Most common minerals in decreasing order of appearance
Fracture properties (DFN description and other properties)	All defined fracture sets can have different properties.
Intensity	Numeric; given as intensity measure P_{32}
Clustering	Spatial correlation of fractures (model)
Size	Equivalent radii
Width	Numeric (indicative)
Filling	Dominant mineral
Surface roughness: A	Stepped, Undulating, Planar
Surface roughness: B	Rough, Smooth, Slickensided
Weathering	Classification in terms of *fresh* and different degrees of *weathering*
Aspect ratio	If fracture shapes are defined as ellipses
Number of sides	If fracture shapes are defined as polygones
Direction of elongation	If fracture shapes are defined as ellipses
Fracture termination	
Fracture set orientation	

Deformation zones	Can be defined with the same set of parameters as rock (see above), with additional, unique parameters below.
Orientation	
Slipvector	Orientation and slip length, if applicable
Length	Applies to the surface trace length of the zone
Thickness	
Geometric uncertainty	

3.3 Hydrogeological modelling

3.3.1 Hydrogeological objects

The Hydrogeological Site Descriptive Models are based on the corresponding geological models, and on discipline-specific methods such as analyses of hydraulic single-hole tests and interference tests. The resulting description consists of hydrogeological properties assigned to geometrical units called *Hydraulic Conductor Domains (HCD)* and *Hydraulic Rock Domains (HRD)*, see Figure 3-2. A description of the soil cover in terms of *Hydraulic Soil Domains (HSD)* is also devised.

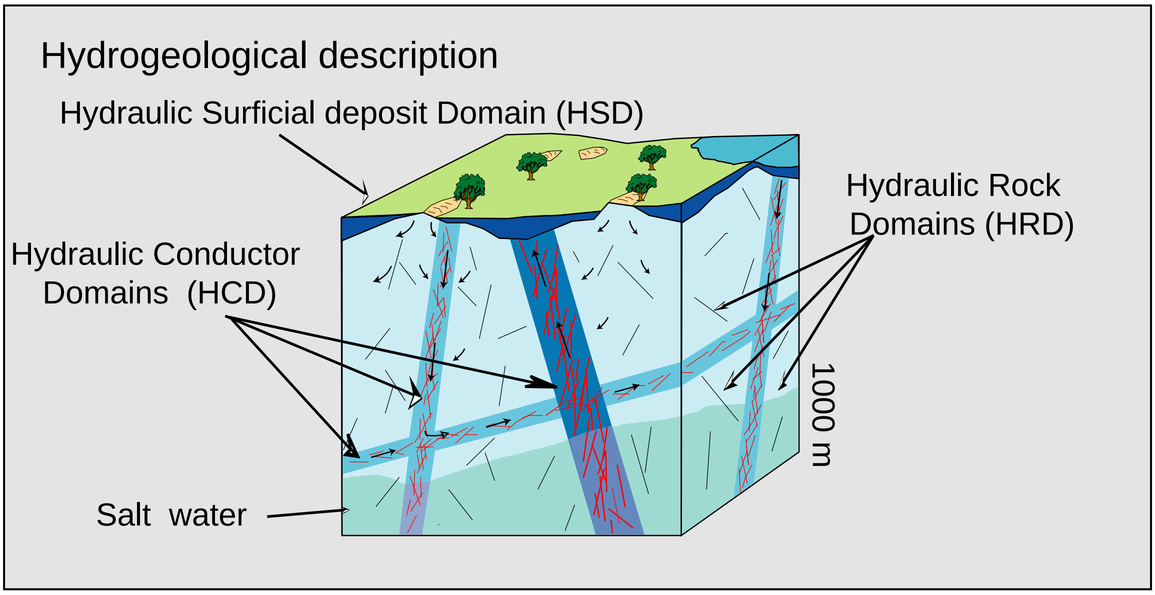


Figure 3-2. *Principal illustration of the main features of a hydrogeological model /from SKB, 2001b/.*

The aim is that the structures that are described deterministically (with respect to their geometrical descriptions) in the geological model, that is, Regional, Local major and some Local minor fracture zones, are to be described as HCD in the hydrogeological models. It follows that the stochastic fractures and fracture zones will be contained within the HRD. However, this association of deterministic structures is possible only if it can be verified that the structures defined by Geology also can be identified as (water-)conductive structures (or otherwise of importance, e.g. as barriers) in the model developed by Hydrogeology. In the hydrogeological modelling, primary hydrogeological data (e.g. from hydraulic tests and flow logging in boreholes) are used in conjunction with the geological description to develop a description of the features that are conductive or otherwise important for the groundwater flow within the model volume /see Rhén et al, 2003/.

3.3.2 Hydrogeological parameters

The hydrogeological parameters assigned to deterministically modelled fracture zones include storage coefficients (for transient flow simulations) and deterministic values or stochastic distributions of transmissivities or hydraulic conductivities. For the stochastic fractures and fracture zones, the descriptions contain different parameter sets for the different modelling approaches to be applied in numerical groundwater flow modelling. Specifically, stochastic distributions of hydraulic conductivities and storage coefficients are provided as input to stochastic continuum (SC) models, whereas statistical descriptions of spatial distributions, geometric properties and transmissivities of structures are provided for use in discrete fracture network (DFN) models; these concepts are further described below. The hydrogeological parameters are summarised in Table 3-3, which is based on the hydrogeological modelling strategy report /Rhén et al, 2003/.

Table 3-3. Parameters in the hydrogeological description /from Rhén et al, 2003; Tables 3-1, 3-2, 3-3/.

Parameters, notation [dimensions]	Description scale (m)	Spatial representation	Comment
HCD parameters			
Transmissivity, *T* [L^2T^{-1}]	10–100	Constant or stochastic distribution within HCD	One deformation zone may consist of several HCDs.
Storage coefficient, *S* [–]	10–100	Constant or stochastic distribution within HCD	Generally assumed to be a function of *T.*
Total width of zone (formation thickness), *b* [L]		Constant within each domain	Based on joint geological-hydrogeological analysis.
HRD parameters – DFN			
Transmissivity, *T* [L^2T^{-1}]	(1–100)	Stochastic distribution within HRD	
Storage coefficient, *S* [–]	(1–100)	Stochastic distribution within HRD	Generally assumed to be a function of *T.*
Total width of feature (formation thickness), *b* [L]		Constant within each each feature	Based on joint geological-hydrogeological analysis. Generally assumed to be a function of *T*.
HRD parameters – SC			
Hydraulic conductivity [LT^{-1}]	5, 20, 100	Constant or stochastic distribution within HRD	
Specific storage coefficient [L^{-1}]	(5, 20, 100)	Constant or stochastic distribution within HRD	Generally assumed to be a function of *K.*
Specific yield [–]	(100)	Constant or stochastic distribution within HRD	

Table 3-3 presents the basic hydrogeological parameters to be assigned to HCDs and HRDs. In addition, DFN models are developed as a part of the three-dimensional modelling within Hydrogeology. Depending on the outcome of the joint geological-hydrogeological analyses, these DFN models of the conductive features may or may not deviate from the descriptions of the corresponding total fracture populations delivered by Geology.

The DFN description of the conductive features is expressed in terms of the same parameters as the geological DFN description (intensity, clustering, size, width, etc; see Table 3-2). However, the parameter values may be different, because the conductive features are a subset of the fracture population identified by Geology. Furthermore, Hydrogeology assigns hydrogeological parameters (transmissivity and storage coefficient) to the conductive features. The analysis of DFN hydraulics is described by /Rhén et al, 2003/.

3.3.3 Groundwater flow modelling

The Hydrogeology programme will develop numerical groundwater flow models to be used for purposes of data interpretation and parametrisation, and in simulations for describing flow rates and flow paths to be used within other disciplines and Safety Assessment. In particular, particle-tracking simulations in groundwater flow models is the basis for quantification of flow-related transport parameters. Different modelling approaches and codes will be used in this work.

As indicated above, conceptual models and modelling tools for groundwater flow in fractured rock can be divided into two basic categories: Stochastic Continuum (SC) and Discrete Fracture Network (DFN) models. These concepts are illustrated in Figure 3-3. In a SC model, data from hydraulic tests in boreholes is used to develop a continuum description of the hydraulic conductivity field. The relation between measurement and model scales is important for the parametrisation; usually, empirical relations are used for upscaling borehole conductivity data. Fracture data is not used directly in these models, but can be used as part of the interpretation basis for obtaining properties in the continuum model. Thus, the SC flow models for fractured rock are similar to the groundwater models for unconsolidated porous media. The large degree of heterogeneity that usually characterises a fractured medium is embedded in the continuum description.

In a DFN model, stochastic and deterministic fracture data is used to generate a fracture network, that is, a geometric description of fractures and fracture zones with hydraulic properties assigned to the conductive structures. Groundwater flow modelling is performed in a second step, either directly in the network formed by the conductive structures or in a simplified "equivalent network", e.g. a set of pipes or channels that in some respect correspond to the DFN. Thus, the DFN models make direct use of fracture data and provide realisations of fracture networks that reflect the available information on the geometry of structures where flow takes place.

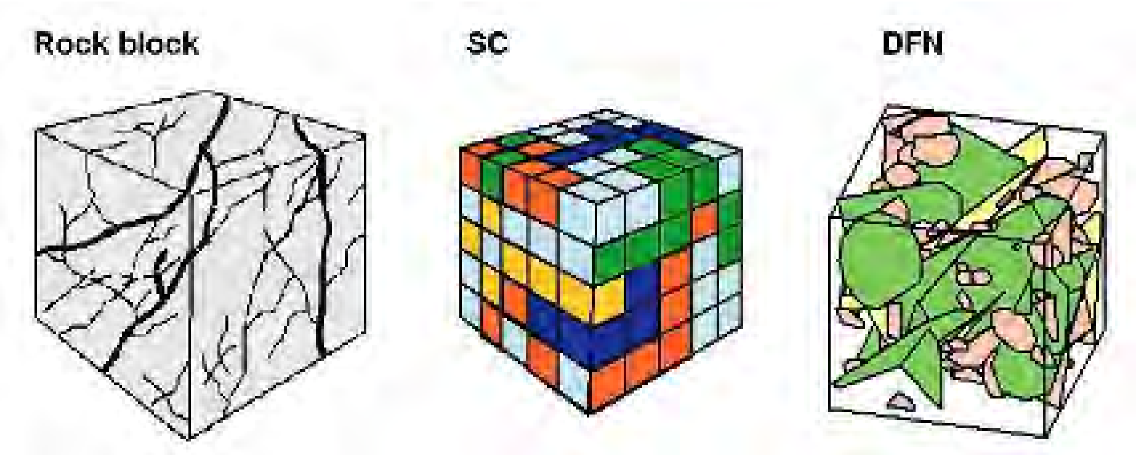


***Figure 3-3.** Schematic view of the Stochastic Continuum (SC) and Discrete Fracture Network (DFN) modelling approaches /from Rhén et al, 2003/.*

A number of different groundwater flow models will be used during the Site Investigations. Two codes have been selected as the main simulation tools:

- DarcyTools /Svensson et al, 2004; Svensson and Ferry, 2004; Svensson, 2004/.
- CONNECTFLOW /Hartley and Holton, 2003; Hartley et al, 2003a,b/.

These codes combine the SC and DFN approaches in different ways. In DarcyTools, developed and described by /Svensson et al, 2004/, a continuum description is developed based on a DFN. This implies that “equivalent continuum parameters” are calculated in the DFN and then are used to parametrise the elements in the continuum model. Thus, parameters such as hydraulic conductivity and porosity are evaluated from fracture data and transferred to the continuum. Unlike “classical” SC models, the fracture data is included in the model and can be used as a basis for computing also other parameters (e.g. parameters of relevance for transport modelling). This approach can be referred to as a mixed DFN/Continuum approach.

The main constituents of the CONNECTFLOW model are the continuum code NAMMU and the DFN code NAPSAC (see /Hartley and Holton, 2003; Hartley et al, 2003a,b/ for documentation of the codes in the CONNECTFLOW package). Combined continuum and DFN models can be developed, which makes it possible to have a detailed DFN model nested within a larger continuum model. Also in CONNECTFLOW, continuum parameters can be calculated from a DFN to obtain a more direct link between fracture data and the continuum model than in “classical” SC models. Other groundwater flow codes that may be used during the Site Investigations are SC models such as GEOAN /Holmén, 1997/, and the DFN code FracMan/MAFIC /Dershowitz et al, 1995/. DFN codes, primarily FracMan in “analysis mode”, are also used in the development of primary DFN descriptions within Geology and Hydrogeology.

3.4 Hydrogeochemical modelling

3.4.1 Modelling process and objectives

The strategy for site descriptive hydrogeochemical modelling is presented by /Smellie et al, 2002/; the contents of this section are mainly taken from their report. Figure 3-4 shows a flowchart of the modelling process. The modelling is performed in a step-wise approach that can be applied at different stages of the site investigations. Specifically, the flowchart describes the modelling during the Initial Site Investigation (ISI) stage. Depending on the complexity of the site, additional iterations may have to be considered in the later model versions. However, the main components of the modelling process will be the same as in Figure 3-4. Note, in particular, the blue boxes in the flowchart. They indicate the different types of evaluations to be performed, and thereby also the various output data provided in the model.

The Hydrogeochemical Site Descriptive Model combines a quantitatively-derived hydrogeochemical model (a model based on site measurements) and a qualitatively-derived hydrogeochemical model (a more descriptive, process-oriented conceptual model). The main objectives of the modelling work are to describe the chemistry and distribution of the groundwater in the bedrock and overburden, and the hydrogeochemical processes involved in its origin and evolution. This description will be based primarily on measurements of the groundwater composition, but also incorporates use of the geological and hydrogeological site descriptive models.

Specifically, the scope of the Hydrogeochemical Site Descriptive Model is to understand

- the origin and evolution of the groundwater chemistry,
- the influence of the surrounding lithological types on the groundwater chemistry,
- the influence of the fracture mineralogy (through water/rock reactions) on the groundwater chemistry,
- the influence of hydraulic mixing processes on the present groundwater chemistry,
- the influence of hydraulic mixing processes on the past composition of the groundwater (i.e. palaeohydrogeochemistry),

and to allow assessment of future hydrogeochemical changes at repository depths. Furthermore, together with the hydrogeological modelling, the hydrogeochemical model should establish the basis for predicting short-term (some tens of years) changes in groundwater chemistry resulting from repository excavation and subsequently during open, operational conditions.

As described below, the site descriptive modelling of transport properties will use hydrogeochemical data for identifying adequate hydrochemical conditions in the laboratory experiments, and in the evaluation of model confidence and site understanding. The use of transport data within the hydrogeochemical modelling will be limited, except for as input to fully coupled reactive transport simulations.

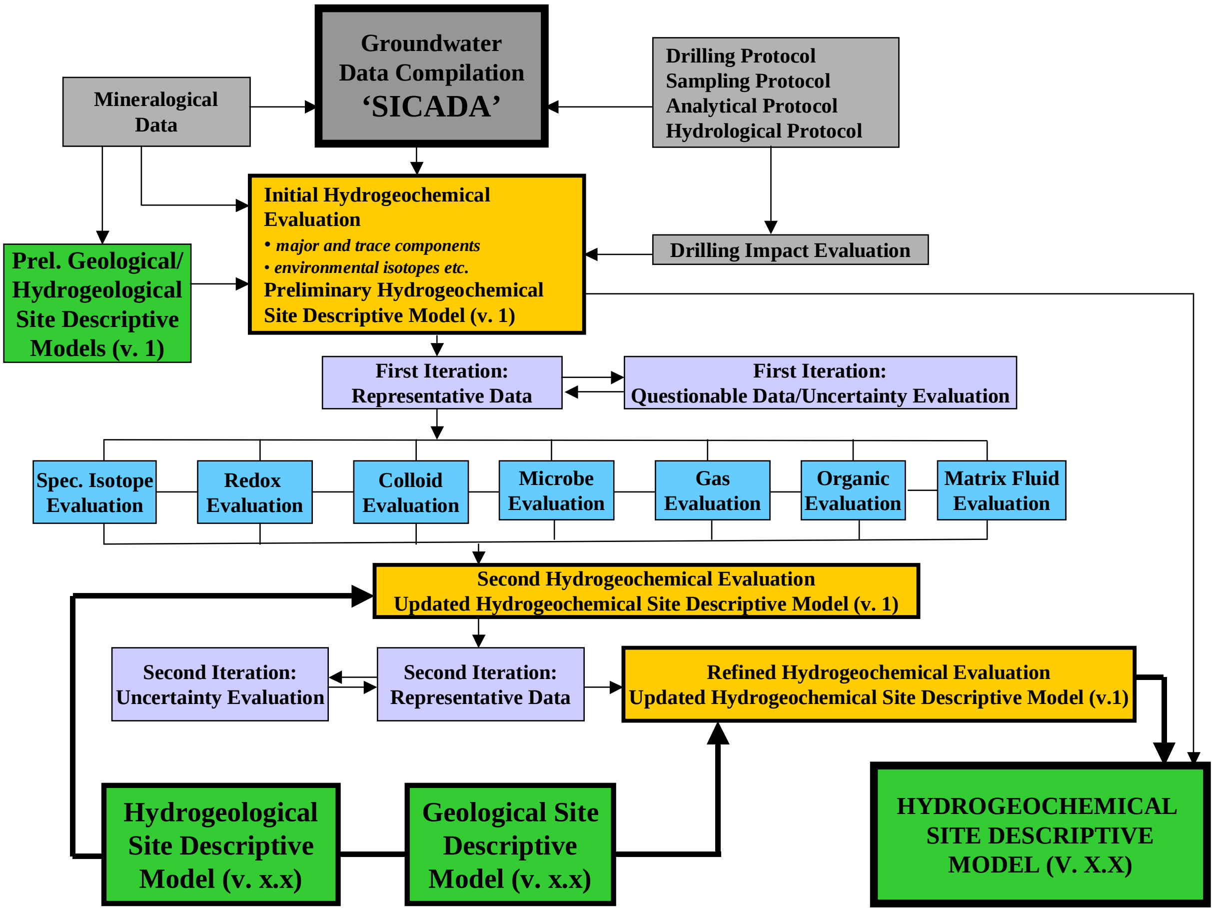


Figure 3-4. *Flowchart showing the site descriptive hydrogeochemical modelling /from Smellie et al, 2002/. The yellow boxes indicate the major stages in the hydrogeochemical evaluation.*

3.4.2 Evaluations and output data

The major output data from the hydrogeochemical site characterisation will refer mainly to chemistry (major ions and trace elements), isotopes (environmental and more specialised types), dissolved gas contents, redox potential conditions, presence of organic material (mainly humics), and populations of colloids and microbes. These data will be related broadly to three major site subdivisions, i.e. surface (surface-based investigations), near-surface (overburden and upper bedrock, down to approximately 100 m) and subsurface (depths > 100 m, information from deep boreholes); alternative subdivisions may be considered, depending on the complexity of the site and the availability of data.

Hydrogeochemical output data, together with available geological and hydrogeological data, will be evaluated and modelled to derive an understanding of the origin and evolution of the different groundwater types. The data interpretation and modelling work consists of an initial hydrogeochemical evaluation, an evaluation of specialised study areas, and, based on additional data that become available from the site investigations, second and refined hydrogeochemical evaluations.

The hydrogeochemical evaluations include:

- Quality control.
- Evaluation of chemical and isotopic trends: depth and lateral variations, time series variations, evidence of water/rock interactions and other reactions, evidence of paleohydrogeochemical trends, and identification and mixing of different groundwater end-members. These evaluations are performed with the aid of various data analysis and plotting tools.
- Hydrogeochemical modelling: two specific hydrogeochemical modelling approaches will be employed to address water/rock interactions and mixing of different groundwater end-members. The PHREEQC code /Parkhurst and Appelo, 1999/ will be used to model water/rock interactions, whereas the Multivariate Mixing and Mass balance (M3) calculations program /Laaksoharju et al, 1999/ will be used to cover end-member mixing processes and an overall statistical appraisal of the hydrogeochemical data.
- Conceptualisation and visualisation: a site descriptive hydrogeochemical model is produced that describes, e.g. the presence and location of major groundwater bodies, variations is hydrogeochemical conditions, and areas influenced/dominated by water/rock interactions, microbially-mediated reactions or mixing. Data interpolations and visualisation tools are used to present the resulting site descriptive model.

Uncertainties will be described and quantified in all steps of the modelling process. The evaluation of specialised study areas includes evaluations of specialised isotopes, redox conditions, colloids, microbes, dissolved gases, organic carbon and matrix fluids (the blue boxes in Figure 3-4).

It follows from the above description that the site descriptive hydrogeochemical modelling presents data on water compositions, and interpretations and modelling results on identified “typical” water compositions and water/rock interaction processes. In addition, a joint geological-hydrogeochemical analysis of the fracture minerals will be presented. The Transport programme (investigations and modelling) will use hydrogeochemical data for three main purposes:

- To identify relevant water types for use in laboratory batch sorption experiments. Identified “typical” water compositions constitute the main hydrogeochemical input to this analysis.
- As input data in the construction of retardation models and for assigning retardation parameters to the geological units in the site descriptive models. Water compositions and fracture mineral analyses are the hydrogeochemical data that mainly will be used for these purposes.
- To assess model confidence and site understanding. These activities will primarily be focused on supporting and alternative/complementary analyses of retention processes. Several types of hydrogeochemical output data will be used in these assessments, including identified water/rock interactions and fracture mineral analyses.

These interactions between Transport and Hydrogeochemistry are further described in Chapter 6 (the retardation model) and Chapter 7 (the three-dimensional modelling).

4 Transport modelling: concepts, processes and parameters

As discussed in Chapter 2, site descriptive transport modelling refers to the process of assigning parameter values to geometric elements and flow paths, whereas conceptual and mathematical transport modelling provides the basic conditions and the analysis tools to be applied in this process. In particular, conceptual and mathematical transport models are important for identifying the relevant parameters to be included in the site descriptive models, as well as for quantifying parameter values.

According to the general conceptualisation of solute transport in fractured rock that is outlined in Chapter 2, the fractured medium is viewed as consisting of mobile and immobile zones. Flow and advective transport of solutes take place in the mobile zone(s), whereas solutes can be retarded or immobilised permanently through interactions with various immobile zones. In addition, transformation processes, such as radioactive decay and hydrochemical reactions, can affect solute transport. This implies that the site descriptive transport modelling requires description/conceptualisation and/or mathematical modelling of the following features and processes:

- The geological conditions along conductive features, including descriptions of different sizes/classes of structures and different types of immobile zones.
- The hydrogeological conditions, groundwater flow rates and velocities, their spatial distributions and temporal variations, and the resulting advective transport.
- The processes governing the mass transfer between mobile and immobile zones, the rates of these processes, and the transport and ultimate retardation/retention capacities within the immobile zones.

In the following, we describe the concepts and mathematical models that constitute the basis for the site descriptive transport modelling, and the parameters to be determined. The emphasis is on models and parameters relevant for radionuclide transport, whereas other transport parameters are discussed briefly in Section 4.7. The emphasis is on the main modelling approach (Chapter 2) with matrix diffusion and sorption as retention processes; other retention models are described in Section 4.4.

4.1 Conceptualisation

In the repository design, it is required that the deposition tunnels and deposition holes do not intersect, and have a respect distance to, regional and local major fracture zones /Andersson et al, 2000/. It is also required that deposition holes are not intersected by identified local minor fracture zones, and a low fracture density is preferred. The individual fractures within the rock mass are thus important for transport, since they will likely act as the first water-conducting transport pathways into the rock barrier from the buffer, in case of a leakage from a defect canister. Since these fractures are small (relative to the fracture zones), and presumably characterised by comparatively low velocities and strong retention, they are important for the overall retention effect of the geosphere.

With time, as transport away from the defect canister proceeds, the released radionuclides reach larger fractures and fracture zones. Thus, it can be expected that the structures where the "water parcels" that carry the radionuclides travel increase in size along the transport path, since structures of large transmissivity (smaller resistance to flow) constitute "preferential paths" within the fracture network. This often implies that flow rates and transport velocities increase with the travel distance from the release point, although large structures sometimes are associated with relatively small gradients and comparatively low flow rates. In either case, the main implication of this schematic transport scenario is that radionuclide transport may take place in features of very different types and sizes, which means that the transport properties of these different features need to be characterised.

Similar to the groundwater flow modelling approaches outlined above, transport modelling can be based on an overall conceptualisation of the fractured medium as either a continuum or as a network of connected discrete features. Models that combine discrete features and continuum descriptions, within or between the features, are also available. In continuum models, the fractured medium is described as an "equivalent porous medium", with appropriately volume- or area-averaged parameters representing the conductive features and the rock mass between the features. In discrete models, the conductive features can be represented as a network of interconnected pipes or channels, or as planar fractures obtained directly from a DFN description.

Solutes are transported by the groundwater flow, that is, by advection, along connected conductive features in the rock (the mobile domain(s)). The solutes are also subject to retention due to interactions between the mobile water and immobile zones along the transport paths. Diffusion and sorption are commonly regarded as the most important processes in these interactions, but also other processes, primarily various homogeneous and heterogeneous hydrogeochemical reactions, can affect solute retention. Depending on the particular solute and immobile zone considered, and the time scale of transport, diffusion and sorption may act as individual processes or in combination. Specifically, non-sorbing solutes are subject to diffusive mass transfer (but obviously not to sorption), whereas some immobile domains (e.g. fracture surfaces) are characterised by more or less instantaneous sorption. Conversely, the retention effect of a particular immobile zone can be considerably enhanced if solutes sorb, or are otherwise retained, within that zone.

Conceptual and mathematical models of solute retardation processes have been developed in many previous studies, see /Bodin et al, 2003a,b/ for reviews of conceptual and mathematical models of solute transport in a single fracture. In particular, model development in connection with tracer tests at various scales /e.g. Winberg et al, 2000; Andersson et al, 2002c/ has provided insights into the existence and roles of different immobile zones. The immobile zones of potential importance for solute transport include immobile pore spaces and outer and inner surfaces associated with:

- **Intact rock matrix:** Unaltered ("fresh") rock mass in rock volumes unaffected by deformations and related alterations of the minerals.
- **Altered wall rock:** Rock adjacent to fracture surfaces showing alteration of one or several mineral types.

- **Fracture coatings:** Minerals grown on fracture walls.
- **Fault breccia:** Rock fragments >2 mm in size, formed by brittle tectonic activity.
- **Fault gouge:** Unlithified fragments of rock and minerals usually including clay minerals found in faults.
- **Stagnant zones:** Immobile water zones within or adjacent to fractures, e.g. dead-end pools, zones of small aperture, or pore spaces where flow is negligible under the local hydraulic conditions at hand.

Additional definitions and more detailed descriptions related to fracture minerals and immobile zones are given by /Widestrand, 2003/. Note that the stagnant zones, their existence, extent and hence their effects on transport, to some extent depend on the local flow conditions, whereas the other immobile zones are identified and described primarily based on geological and hydrogeochemical evidence (analyses of fracture mineralogy and geochemistry).

The conceptual model of immobile zones and transport processes developed within the TRUE Block Scale project is shown in Figure 4-1 /Poteri et al, 2002/. The figure illustrates the micro-scale geology and the active transport processes (under tracer test conditions) along a small section of a conductive feature, as interpreted from characterisation and modelling work conducted during the project.

As discussed above and illustrated in Figure 4-1, spatial variability can affect solute transport in different ways, that is, through variability in different processes and parameters, and on a wide range of scales (see also /Bossart et al, 2001/). Different geological conditions (structures of different types and sizes) are encountered along a transport path through the geosphere. As a result, flow and transport are spatially variable along transport paths. This variability manifests itself as variability in transport properties along individual paths, and, in an integrated sense, as different effects of the transport processes along different paths. Figure 4-1 shows that transport properties can be expected to vary in the transport direction also on a considerably smaller scale. The existence of small-scale variability in sorption and diffusion properties has been verified experimentally by /Xu and Wörman, 1998/ and /Byegård et al, 1998/.

In addition, the existence of different immobile zones, especially the fracture coatings and altered wall rock, implies that the properties governing diffusion and sorption are spatially variable in the direction perpendicular to flow and advective transport. Taking the commonly applied parallel plate model /Neretnieks, 1980/ as a conceptual basis, this means that solute penetration into the rock matrix, and sorption of solutes there, are determined by properties that display spatial variability in the transverse direction (cf. Figure 4-1). Such variability has been observed at Äspö HRL /Byegård et al, 1998/. As mentioned in Section 2.8, transverse variability implies a time dependence of "effective" diffusion and sorption parameters, since the solutes "integrate" matrix of different properties in the process of solute penetration into the rock.

Our ability to describe spatial variability, and to assign relevant parameter values in view of this variability, is a critical aspect of the site descriptive modelling work. Clearly, a complete description of micro-scale variability of all relevant properties within the entire modelling domains is neither achievable nor required. Similar to the descriptions produced by Geology and Hydrogeology, the transport properties modelling will to some extent rely on statistical methods for describing spatial variability. It should also be noted that the present strategy for obtaining sorption parameters is empirical, in the sense that the dependency of the parameters on the hydrogeochemical conditions at the site is handled by performing experiments with different "typical" water compositions. Since only a few water compositions can be included in the experimental programme, this implies that spatial variability in the hydrogeochemistry of the site is a source to uncertainty in the transport description.

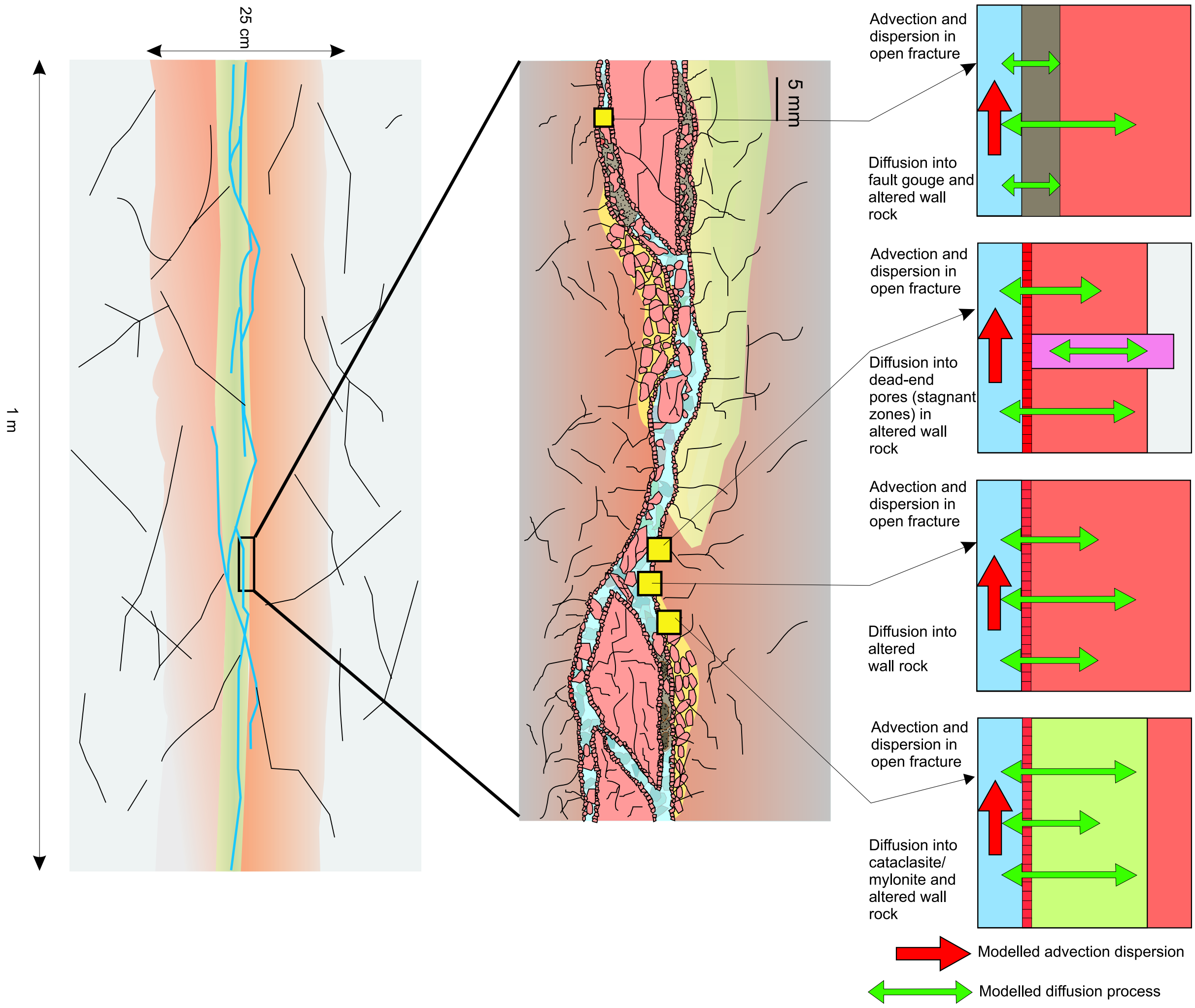


Figure 4-1. *Illustration of pore space structure, immobile zones, and interaction processes /from Poteri et al, 2002/.*

4.2 Mathematical modelling

Since advection is the dominant "carrier" process for solutes in fractured rock, transport modelling is closely related to groundwater flow modelling. Thus, the transport modelling is based on similar basic conceptualisations of the fractured medium as those underlying the flow modelling, that is, the medium is described as a continuum, an "equivalent porous medium", or as a network of interconnected discrete elements that represents the conductive features. As indicated above, transport modelling requires additional descriptions and parameters, related to both advection and retention. In particular, parameters of geometric character are needed to relate flow rates to solute velocities and travel times, and to describe mass transfer and immobile zones.

For the description of solute transport, the following basic conceptualisations can be considered:

- A Eulerian approach where the fluid is viewed as continuous with spatially (and temporally) variable solute concentrations. In this approach, concentrations are calculated as functions of regular Cartesian coordinates (x, y, z).
- A Lagrangian approach where transport is modelled by following solute "particles" or "parcels" as they move with the groundwater velocity through the fractured medium. Transport is here described in terms of coordinates that "follow the particles" (e.g. the travel time between injection and exit locations). Under conditions of steady flow, all particles released at a given point follow the same path through the domain.
- Lagrangian approaches utilising "clusters of sub-particles" where different particles released at the same location may behave differently in response to processes such as diffusional mass transfer and local dispersion, or take different paths due to "branching" at fracture intersections.

It follows that flow and transport models are integrated (coupled) to different extents in different modelling approaches. With respect to the interactions/data exchanges between flow and transport models, the following approaches can be identified:

- Groundwater flow models are used to calculate hydrodynamic transport parameters that are used directly in the transport description, as a description of non-sorbing solute transport, and/or are used as input to separate transport models. These parameters include the water travel time and the "F-factor" (sometimes referred to as "transport resistance", see /SKB, 2001b/). Additional parameters required to describe advection (e.g. flow porosity in SC models) are either handled separately, or are provided as external input or are calculated by the flow codes (DarcyTools). Retention can be modelled in separate models or, in simplifying cases, by scaling of the hydrodynamic parameters. The latter alternative was the main approach used to calculate transport parameters in SR 97 /SKB, 1999a/.
- Groundwater flow models are parameterised with advection and retention parameters, and both hydrodynamic parameters and combined advection-retention parameters are calculated by integration along flow paths (particle tracking). As with the purely hydrodynamic parameters obtained in the approach described above, these parameters may either constitute the full description of transport or provide a basis for further modelling. The existence and identification of relevant integrated parameters is based on analytical solutions of the transport equations. Therefore, this approach (and the previous one) can be termed "semi-analytical". This approach to calculating both advection and retention parameters has been developed and used for evaluating tracer tests within the TRUE programme /Cvetkovic and Cheng, 2002/.
- Coupled flow and transport modelling, which implies that transport modelling is performed by solving mass balance equations for the solutes in discrete elements

within the transport domain, using (local) hydrodynamic data (e.g. velocities) as input. Thus, “actual process modelling” of the advection and retention processes is performed, which requires a complete parametrisation of the model. The elements can be finite elements in a numerical continuum model or discrete structural elements in a DFN model. When implemented within a Eulerian framework, this is the classical approach to numerical transport modelling. Models of this category have been utilised within the TRUE and Äspö Task Force programmes /e.g. Poteri et al, 2002/. A general class of retention processes can be considered (not only those that have analytical solutions), which means that also alternative retention models can be investigated (cf. Section 4.4). Recently, coupled transport-reaction modelling has been performed also within a Lagrangian framework /Malmström et al, 2004/, using PHREEQC to model hydrogeochemical reactions along streamtubes of different travel times.

During the site investigations, transport modelling will be based primarily on particle tracking simulations, in which flow-related parameters are calculated (see Chapter 7). Particle tracking simulations can be performed in both SC and DFN models. However, it should be noted that different flow models generate different types of particle tracking results. For steady flow, particle tracking in SC models result in particle trajectories that also are streamlines. Thus, streamtubes associated with the streamlines will have a constant (along the path) volumetric flow rate. In DFN models, particles will experience different flow rates along a single path. In some cases, these differences are important for, e.g. statistical evaluations.

In either modelling approach, the flow field has the important role of defining the flow and transport paths in the fractured medium, which, in turn, determine which immobile zones will interact with the transported solutes. Essentially, particle tracking identifies collections of paths and parameters associated with these paths. Based on such results from a series of realisations of the medium, a description is to be produced that contains parameter values with relevant measures of spatial variability and uncertainty.

4.3 Main modelling approach

4.3.1 Assumptions

It should be evident from the description above that solute transport in fractured rock takes place in geometrically, geologically, hydrogeologically and hydrogeochemically complex systems, and that a number of different transport processes can affect the fate of released solutes. Consequently, many different modelling approaches can be taken, involving different levels of complexity in the descriptions of the fractured medium, the flow system, and the physical and chemical transport processes. The main approach to radionuclide transport properties modelling in the Site Investigations is based on, and produces output data for, a class of transport models with the following common assumptions:

1. *Decoupling of solute transport and hydrogeochemistry.* Data on the hydrogeochemical conditions are used in the process of sorption measurements and parametrisation of models, but changes in hydrogeochemistry are not modelled explicitly in the transport modelling.

2. *Decoupling of advection and retention processes.* Retention processes that affect flow and advection (e.g. by precipitation and "clogging" of flow paths) are not considered.
3. *Linear and reversible retention processes.* According to the definitions in Section 2.10, this implies the wider class of "retention processes" reduces to "retardation processes". The linearity implies that retardation is independent of solute concentrations and that different processes can be handled separately in the models.
4. *Instantaneous sorption.* Equilibrium sorption conditions are assumed for all inner and outer surfaces.
5. *Steady groundwater flow.* Transient groundwater flow will be modelled during the Site Investigations, but transport parameters will be calculated under conditions of steady flow using "snap shots" of the flow field corresponding to the present situation.

These assumptions could be relaxed in sensitivity studies during the Site Investigations, primarily in the context of assessing site understanding and model confidence. However, it is foreseen that such studies, especially quantitative modelling, will be performed mainly in the framework of Safety Assessment.

4.3.2 Processes and parameters

Some of the important features of solute transport in fractured rock are described in the preceding sub-sections and in the overview in Chapter 2. The main transport processes are there described in a qualitative manner, without rigorous definitions or mathematical equations. In the following, a description of the individual processes and some basic notation is given. For a more detailed account of transport processes in a SA perspective, see the SR 97 "Process report" /SKB, 1999b/.

Advection and dispersion

Advection is defined as transport with the flowing groundwater, that is, as transport with the (bulk) movement of the groundwater. In most cases of practical interest, advection is the main "carrier" process for solutes in the groundwater. This implies that advection is usually the most important process to describe in connection with solute spreading. It follows from the definition that the rate of advective transport is proportional to the flow velocity and to the solute concentration in the water. Thus, the quantification of advection is strongly linked to groundwater flow modelling, such that calculated **fluid velocities** is the only input required for transport calculations. However, when using continuum flow models that produce Darcy velocities as output, the **flow porosity** is required to quantify advection (cf. below).

Dispersion should be regarded as a concept, rather than as a process or a parameter. In classical advection-dispersion models for solute transport, dispersion accounts for solute spreading at scales smaller than the one associated with the advection process. Molecular diffusion and spatial variability in the velocity may both contribute to the dispersion; however, dispersion is usually dominated by the velocity variations. This means that the groundwater velocity in advection-dispersion models is separated into advection and dispersion components. Although dispersion is dominated by velocity variations, it is described as a diffusion process in these models.

In a one-dimensional advection-dispersion model, the longitudinal dispersion can be represented by a **dispersion coefficient,** D_L **[**L^2T^{-1}**]**, a **dispersivity** α_L **[L]**, or as a

dimensionless Peclet number, *Pe* ($Pe \equiv V L / D_L$) where V is the velocity and L is the length scale. Thus, advection-dominated conditions correspond to large *Pe*, whereas (very) small *Pe* indicate that diffusion is important for dispersion and solute transport in the mobile zones. It is well known from experimental observations and theoretical analyses that dispersion is scale-dependent. This implies that the concept of dispersion as a large-scale transport process is somewhat difficult to implement, especially if different transport distances are to be considered, and/or in connection with spatial variability in other processes than advection. The main alternative to the classical dispersion approach is to describe spatial variability in solute velocities or travel times explicitly, as, e.g. travel time distributions.

Combinations of dispersion (modelled as diffusion) and spatially variable velocities or travel times may also be appropriate in some cases. For example, a dispersion concept is often used to model sub-grid variability in numerical models. Furthermore, "numerical dispersion" arises in numerical transport models, which may set a lower limit for the modelled effect of dispersion that depends on the resolution of the model.

Diffusion

Whereas molecular diffusion within the mobile zones is generally of secondary importance, diffusion is usually considered an important process for mass transfer between mobile and immobile zones, and for the subsequent transport within immobile zones of such spatial extent that transport shows non-negligible transients (e.g. in the rock matrix). As discussed above, diffusion is considered an important process for radionuclide retention in fractured rock. However, similar interactions may also be important for the modelling of density-dependent groundwater flow, and for hydrogeochemical modelling.

Mass transfer concepts, where the models are parameterised by lumped resistance parameters, are often used to describe physical rate limitations offered by "thin" layers of immobile water adjacent to solid phases, and in models that contain stagnant zones /e.g. Poteri et al, 2002/. In linear mass transfer models, diffusion is parametrised by use of **mass transfer rate coefficients $[T^{-1}]$** and parameters that quantify the capacities of the immobile zones (their maximum contents of immobilised solute mass). In the groundwater flow and transport model DarcyTools, see Section 3.3.3, coupled solute transport and density-dependent flow can be modelled by a linear "multi-rate approach", such that different immobile zones can be parametrised by different sets of rate and capacity parameters.

Diffusion into and within the rock matrix is generally treated as a transient process, where diffusive transport is modelled by solving diffusion equations. This requires a geometric description of the diffusion domain(s), as well as specifications of initial and boundary conditions. In many cases, a parallel plate model /Neretnieks, 1980/ is applied in models for matrix diffusion. This means that diffusion is assumed to take place in a one dimensional domain perpendicular to the flow direction in the fracture. This domain can be modelled as infinite or finite, where "outer boundaries" could be associated with other fractures in a dense fracture network.

The diffusion properties of the matrix can be expressed in terms of the **effective diffusivity, D_e $[L^2T^{-1}]$**, or the **pore diffusivity, D_p $[L^2T^{-1}]$**. These parameters are related as $D_e = D_p \theta_m$, where **θ_m [–]** is the **porosity of the matrix**. Strictly, the relevant porosity to be used in this context is the "effective porosity" for the diffusion process, which may differ from the total matrix porosity. Different materials/zones (e.g. intact rock and altered rim zone) often have different diffusivities and porosities, and these parameters can also be spatially variable within each zone. In addition, different solutes have different diffusivities, and the diffusivities also depend on the chemical composition of the water (see /Widestrand et al, 2003/ for a description of how this is handled in the laboratory programme).

Based on experimental observations, it has also been suggested that different diffusion mechanisms need to be considered when modelling matrix diffusion. In particular, surface diffusion within a sorbed phase, quantified by a separate diffusion coefficient, has been included in some diffusion models /e.g. Ohlsson, 2000/. Results of diffusion experiments are sometimes expressed in terms of an "apparent diffusivity". In these cases, the relation between the "apparent diffusivity" and D_e or D_p is often used to quantify additional sorption and/or surface diffusion parameters.

The **formation factor, F_m [–]**, is used as a non solute-specific, dimensionless representation of the diffusivity /Ohlsson and Neretnieks, 1997/; this parameter will be the basis for assigning diffusivities to different radionuclides in the SI laboratory programme /Widestrand et al, 2003/. It is defined as $\boldsymbol{F_m = D_e / D_w}$, where $\boldsymbol{D_w}$ **[L^2T^{-1}]** is the solute diffusivity in water. Thus, F_m is a geometric parameter, which accounts for the fact that only a small fraction of the pore space available for diffusion and for the additional resistance arising due to tortuosity and reduced connectivity in the pore system. Since D_w in many cases is available from previous experiments (literature data), the effective diffusivity can be calculated if F_m can be measured or calculated. Several constitutive equations are available that relate the formation factor to various geometric and other parameters /see, e.g. Löfgren and Neretnieks, 2002/.

Diffusion is a physical process that occurs in any medium in presence of a concentration gradient. It is commonly agreed that matrix diffusion is important for radionuclide retention, and it is usually included in performance assessment modelling of waste repositories in fractured rock. However, some issues related to the quantification of matrix diffusion are still debated within the scientific community. Essentially, these issues concern the persistence of the process in space and time, especially the implications of variability and uncertainty related to spatial and temporal dependencies for the parametrisation of transport models. Specifically, there exist somewhat different views on the extent of the connected pore space outside fractures, and hence on the matrix volume available for diffusion and sorption (see discussion on porosity below).

Potential future changes in the effect of matrix diffusion are related to processes on fracture surfaces, such as precipitation, that may change the accessibility to the matrix through "pore clogging". The potential for these processes to occur can be assessed based on detailed predictions of the hydrogeochemical development of the investigated site. The present modelling strategy for diffusion is based on laboratory measurements of the diffusion coefficient, complemented by in situ measurements and geological and hydrogeochemical data (see Chapter 5). Matrix porosity and diffusion parameters are also affected by the differences in stress conditions between the intact rock mass and the samples used in laboratory experiments. The effects of this stress release are considered in the data evaluation /see Widestrand et al, 2003/.

Porosity

The fractured rock is viewed as a dual porosity medium, where the primary porosity is associated with the fractures and fracture zones, and the secondary porosity is within the immobile zones, primarily the rock matrix. This means that the medium contains different types of pore spaces, which are relevant for the transport description at different scales and for different transport processes. Note that the matrix porosity usually is much larger (say, one order of magnitude) than the porosity associated with the (water)conductive fractures. This implies that the volume where retention may take place is very large, compared to the volume available for flow and solute transport.

In continuum models for groundwater flow, the fractured rock is modelled as an "equivalent porous medium". Results of flow simulations are obtained in terms of Darcy velocities (volumetric flow rate per unit total area), which implies that the porosity, a measure of the water volume per unit total volume of the medium, is needed to calculate groundwater velocities and travel times from the Darcy velocities. In this case, the porosity is a macroscopic parameter that quantifies the volumetric fraction of conductive fractures and fracture zones in the medium, similar to the pores in a model for a porous medium.

The macroscopic porosity relevant for evaluation of groundwater velocities and advective transport is determined by the volume of the conductive features where flow takes place. This porosity is referred to as **flow porosity** or **effective porosity**. This parameter is often estimated based on fracture information. If a DFN description is available, the flow porosity can be calculated from the geometric fracture data. Such calculations are performed in the transformation from DFN to SC in DarcyTools (see Section 3.3.3). However, tracer tests are required for a detailed analysis of the relation between flow rates and transport velocities. It should be noted that the effective (flow) porosity depends on the flow conditions, and that it can be different under, for example, different boundary conditions for flow.

Also the secondary porosity in the rock matrix contains different pore spaces that may or may not be relevant for the transport processes that take place there /e.g. Andersson et al, 2002c/. In particular, matrix diffusion is determined by an **effective matrix porosity** comprised by the connected pore spaces, whereas some laboratory methods determine the **total matrix porosity**. In the site descriptive modelling, measured porosities are judged in view of the methods employed, with the aim to report parameter values that are relevant for diffusion. It is assumed that θ_m in the equations below represents an effective matrix porosity for the retention processes. No other general notation for flow- and retention-related porosities is given here; parameters are introduced below, as needed.

It should be noted that the matrix porosity is a parameter that primarily will be handled by the Geology programme. The porosity, however, is strongly related to solute retention, especially to diffusion, and it is obtained as a "by-product" in laboratory measurements of transport parameters. These measurements are important for sample characterisation. From a modelling point of view, it is also important to investigate correlations between different parameters, which means that they should be measured on the same samples/ materials, and to provide a basis for evaluating alternative parametrisations. Therefore, porosity will be measured and described also by Transport.

Furthermore, studies of the connected porosity in the vicinity of conductive features, and the associated time-dependence and ultimate capacity of the retardation processes, may provide important information for the geoscientific understanding of the sites as well as for SA. For example, recent field investigations at Grimsel Test Site indicate that connected porosity can extend to significant depths /Möri et al, 2003/. Under such conditions, retardation parameters for intact rock could underestimate the retention effect also at the SA time scale. There is some field evidence also from Swedish sites indicating large penetration depths for diffusion in rock (on the order of several decimeters, see /Birgersson and Neretnieks, 1990; Löfgren and Neretnieks, 2003/). Laboratory experiments have shown a relatively strong dependence of diffusion on the length of the tested core samples (decreasing diffusion coefficients with increasing sample lengths) on the scale of a few centimeters /Byegård et al, 1998/. This dependence will be investigated also during the Site Investigations /Widestrand et al, 2003/.

Sorption

Sorption includes a number of processes/mechanisms by which solutes become attached to surfaces in the fractured medium, see Section 4.4.2. These surfaces can be outer surfaces on, e.g. fracture walls or breccia fragments, or inner surfaces within the rock matrix. The most important sorption mechanisms are generally ion exchange and surface complexation. However, these mechanisms are not to be modelled explicitly in the present transport properties modelling context. Rather, the assumption of linear equilibrium sorption implies that sorption can be represented by distribution coefficients that directly relate the concentrations in the aqueous phase to the corresponding sorbed concentrations.

It is well known that the sorption of a particular solute depends on the geochemical properties of the surfaces where sorption takes place and on the hydrochemistry of the solution. During the Site Investigations, these dependences will be handled mainly empirically, that is, by performing laboratory experiments on site-specific geological materials and with different water compositions that are identified as typical for (different parts of) the sites. Other methods for capturing the dependence of sorption on the hydrogeochemical conditions are described in Section 4.4, where also retention processes other than sorption are discussed.

In the main modelling approach, surface sorption is expressed in terms of a surface area-normalised distribution coefficient, $\boldsymbol{K_a}$ **[L]**, and sorption in the matrix by the volumetric distribution coefficient $\boldsymbol{K_d}$ **[$\mathbf{L^3M^{-1}}$]**. These parameters can be spatially variable, and can have different values for different solutes and water compositions. Therefore, additional notation (e.g. indices) is usually required. In models that consider multiple immobile zones, also the sorption parameters associated with the different zones need to be distinguished from each other.

In transport models, linear equilibrium sorption can be represented by dimensionless “retardation factors”, whereby the effect of sorption is manifested as a simple temporal scaling. Whereas the retardation factor for surface sorption depends on the geometric description of the transport domain, and hence is model specific, the retardation factor in the matrix can be expressed in a general manner as $\boldsymbol{R_m = 1 + \rho K_d / \theta_m}$, where ρ is the bulk density of the rock material. Note, however, that in cases where the individual parameters are spatially variable, this variability needs to be considered when calculating spatially variable retardation factors.

4.3.3 Flow-related transport parameters

Characteristic parameter groups

A theoretical background to the calculations of flow-related transport parameters is given in Appendix A. Essentially, the transport domain in the fracture system is viewed as a collection of three-dimensional flow paths, which are obtained from particle trajectories in particle-tracking simulations with groundwater flow models. Transport properties are spatially variable along individual flow paths, such that integrated, "effective" transport parameters vary among the different flow paths. Spatial variability is modelled stochastically, which implies that input and output parameters are expressed in terms of random space functions and probability density functions.

Neglecting local dispersion, the solution to the equations for advection, surface sorption and diffusion and sorption in the matrix along an individual flow path, can be expressed as sums of random components along the flow path:

$$t_w = \sum_{i=1}^{N} t_{w,i} \; ; \qquad A = \sum_{i=1}^{N} A_i \; ; \qquad B = \sum_{i=1}^{N} B_i \tag{4-1}$$

where t_w [T] is the water residence time, A [T] is a surface sorption parameter group, and B [$T^{1/2}$] is referred to as "total transport resistance" /Cvetkovic and Cheng, 2002/. The index "*i*" denotes either a fracture, if the particle is transported through a series of internally homogeneous fractures, and/or discretisation segments if we consider single or series of heterogeneous fractures; N is the total number of fractures/segments.

If each segment is characterised by a velocity V_i, length l_i, and half-aperture b_i, then the characteristic advection and surface sorption parameters are defined as

$$t_w = \sum_{i=1}^{N} \frac{l_i}{V_i} \; ; \qquad A = \sum_{i=1}^{N} K_{a,i} F_i \; ; \qquad F_i = \frac{l_i}{V_i b_i} = \frac{t_{w,i}}{b_i} \tag{4-2}$$

where F_i [TL^{-1}] is referred to as "hydrodynamic transport resistance", or "transport resistance" /SKB, 2001b/; here we use "*F*-parameter" to denote this parameter group. If diffusion and sorption parameters θ_m, D_e and R_m for the matrix are assumed uniform within fractures (segments), but can vary among segments, then B can be expressed as

$$B = \sum_{i=1}^{N} M_i F_i \; ; \; M_i = \sqrt{\theta_{m,i} D_{e,i} R_{m,i}} = \sqrt{\theta_{m,i} D_{e,i} \left(1 + \frac{K_{d,i}\rho}{\theta_{m,i}}\right)} \tag{4-3}$$

where M_i is referred to as "material parameters group". In cases where different discretisations/resolutions are used for describing, for instance, advection and retardation parameters, index "*i*" refers to the smallest scale of resolution.

If the retardation parameters are uniform (constant) in the entire transport domain, then

$$A = K_a F \; ; \quad B = M\,F \; ; \quad M = \sqrt{\theta_m D_e R_m} = \sqrt{\theta_m D_e \left(1 + \frac{K_d \rho}{\theta_m}\right)} \; ; \quad F = \sum_{i=1}^{N} F_i \tag{4-4}$$

which implies that only t_w and F must be obtained by integration along the trajectories, and that only the integrated "*F*-parameter" is required for quantifying the "total transport resistance" (not the integrated product of F_i and other parameters). Alternative formulations and possible simplifications of the expressions for the flow-related parameters are described in Appendix A.

Conclusions and guidelines for calculating flow-related parameters

Based on the preceding discussion, and previous analyses /Andersson et al, 1998; Cvetkovic et al, 2000; Lee et al, 1990/, the conclusions and general guidelines for calculations of flow-related parameters in the site descriptive modelling can be summarised as follows:

- Analytical solutions can be obtained for dispersion-free systems. These solutions can be expressed in terms of characteristic parameter groups quantifying advection, surface sorption, and matrix diffusion and sorption. These parameter groups vary among flow paths depending on the spatial variability in flow and retardation parameters.
- Spatial variability along the flow/transport paths can be handled by integrating the characteristic parameter groups along particle trajectories identified through groundwater flow modelling. In view of the stochastic description of spatial variability, the task is to estimate the statistics of the characteristic parameters.
- Different formulations of the parameter groups are obtained for different basic (geometric) descriptions of the flow paths, and for different definitions of retardation parameters. Different modelling approaches and values of geometric parameters should be considered during the Site Investigations.
- The adequate characteristic parameter groups associated with a particular modelling approach or case of spatial variability must be preserved in integrations, statistical evaluations and “extractions” of individual parameters from the parameter groups /cf. Andersson et al, 1998/. Integrations of individual parameters and calculations of parameter groups in post-processing are generally not equivalent to integrations of the whole parameter groups.

4.4 Other approaches to retention modelling

4.4.1 Process-based retention models

As described in some detail above, the main modelling approach for radionuclide retention in the site descriptive modelling (and in SA) is based on matrix diffusion and linear equilibrium sorption. This implies that the contribution from the hydrogeochemical processes to the overall radionuclide retention is modelled by means of K_d-values. These K_d-values are obtained in laboratory experiments using different tracers/nuclides, site-specific geological materials and different water compositions that are relevant for the site conditions. Thus, although the K_d-values provide a lumped quantification of a number of individual processes, the significance of the site conditions for hydrogeochemical retention is quantified empirically in this approach.

Transport models often use the K_d concept to describe sorption, primarily because of its simplicity and computational efficiency. The latter argument is of particular relevance in a performance assessment context, where often a large number of calculations are performed. In addition, the vast majority of radionuclide sorption experiments in the past have been interpreted with K_d-based models. This means that available databases and model experiences to large extent concern K_d-values and K_d-based transport models.

However, the predictive capabilities of K_d-based models have been questioned, especially in the context of long-term performance assessment scenarios with evolving hydrogeochemical conditions, thereby calling for process-based models describing and quantifying the hydrogeochemical interactions between dissolved tracers/nuclides and rock/fracture materials /NEA, 2001/. In the following, a brief description of such models is given; this description is based primarily on /Malmström, 2004/.

Generally, process-based models are expected to have a larger predictive capability and to apply over a wider range of hydrogeochemical conditions than K_d-based models. Process-based models can be used to formulate "mechanistic" sorption models (sometimes referred to as TSM, thermodynamic sorption models). They may also cover additional processes such as precipitation and co-precipitation, which do not occur at the conditions and the short time scales over which conventional laboratory sorption experiments are carried out. In addition, such models handle the dependence of radionuclide sorption/retention on ionic strength, pH and speciation (e.g. hydrolysis and formation of soluble complexes), as well as effects of surface saturation and competition for surface sites /e.g. NEA, 2001/.

Although essentially the same modelling tools (e.g. PHREEQC; Parkhurst and Appelo, 1999) and input data could be used to cover the full range of processes that contribute to hydrogeochemical retention, it is useful to distinguish between:

1) process-based modelling of sorption processes; and
2) process-based modelling of hydrogeochemical retention processes other than sorption.

These two modelling activities are discussed below. The next step in a development towards incorporation of process-based retention models into performance assessment calculations is to couple process-based hydrogeochemical retention models to physical transport models (models that account for transport by advection and diffusion). Such coupled models are not further discussed here.

4.4.2 Process-based modelling of sorption

Sorption processes involve ion exchange onto permanently charged surface sites and surface complexation onto variably charged surface sites on minerals. These processes can be regarded as conceptually relatively well understood on the laboratory scale /e.g. NEA, 2001/. In principle, one can envisage two conceptually and operationally different ways to quantify the processes /Malmström, 2004/:

i. through *site-specific process-based models* building on mechanistic interpretations of trace element sorption onto site-specific mixtures of minerals; and
ii. through *building-from-first principles*, using site-specific, primary geochemical information, such as mineralogical compositions and specific (reactive) surface areas, in conjunction with "generic" sorption models and databases for pure mineral phases from the literature.

Whereas the latter approach is more general, it requires more input data and is associated with a number of conceptual difficulties, such as the determination of exposed surface area and its partitioning into different minerals and mineral faces, as well as the variable sorption behaviour associated with different sites and faces. The former approach provides a site-specific integrated measure of the sorption and thus does not suffer from these conceptual difficulties. On the other hand, it is less mechanistic and not general, and therefore has lower predictive and interpretative capabilities. Employment of any process-based model in field-scale applications requires upscaling of the laboratory quantifications of processes, which in itself represents a conceptual difficulty.

4.4.3 Other retention processes

Processes other than sorption that may contribute to hydrogeochemical retention include precipitation, surface precipitation and co-precipitation. Whereas precipitation processes are well understood and commonly quantified by geochemists using standard modelling tools and databases, surface precipitation and co-precipitation are less well understood. However, quantification methods for co-precipitation (e.g. /Bruno et al, 1995, 1998/; see also summary in /Bruno et al, 2001/) and surface precipitation /e.g. Zhu, 2002/ have been proposed and employed in the literature, and could thus be used and further tested in the present context.

A common motivation for the exclusion of these processes from quantitative analyses of retention is that they provide additional retention capacity, implying that their exclusion is conservative. However, this argument is not valid in the site descriptive modelling context, and it has also been argued that the conservativeness may not be general. Specifically, precipitated radionuclides may be dissolved in connection with changes in the hydrochemistry of the system, thereby possibly creating higher concentrations than predicted with sorption-based models. However, analyses of this type of future scenarios will be handled within the SA framework.

4.4.4 Use of process-based retention models

The hydrogeochemistry of trace elements is commonly affected by major component chemistry through pH and speciation effects. Although extensive thermodynamic databases are available for aqueous phase geochemistry and many pure solid phases, all process quantifications are associated with uncertainty, in particular those associated with trace elements /e.g. Bruno et al, 1998; 2002/. Furthermore, there is limited thermodynamic data available on surface speciation and complexation reactions. This implies that model input inevitably is associated with significant uncertainty already with respect to parameter values.

Generally, current performance assessment models do not include process-based retention models. The main reasons for this are, as mentioned above, the large amount of input parameters required and the difficulties associated with determining some of these parameters, the difficulties related to upscaling from the laboratory to the field scale, and the computational effort required to solve non-linear, multi-component transport-reaction systems. Thus, the K_d-based approach is the main approach to retention modelling in the present strategy and the planned SA calculations, whereas process-based models are considered to need further development before they can be implemented in this context. However, development of process-based retention models is a highly active research area, within SKB and elsewhere, and the modelling framework will likely be revised or complemented in the future.

Although the quantitative analysis of radionuclide retention will be based on the K_d concept, there are important implications and applications of joint hydrogeochemistry-retention analyses in the site descriptive transport modelling. In particular, process-based conceptual and mathematical models will be useful in the assessment of site understanding and model confidence. For example, such models can be used in supporting evaluations of sorption parameters (i.e., comparisons between measured and calculated K_d-values), and for explaining variability in experimentally derived parameters, see Section 7.5. Hydrogeochemical data can also be used to provide site-specific evidence for the retention processes in the descriptive model /see Landström et al, 2001/.

4.5 Transport modelling in Safety Assessment

SKB uses the code FARF31 for modelling radionuclide transport in the geosphere within the Safety Assessment “model chain”. The code was originally described by /Norman and Kjellbert, 1990/; a recent user’s guide is also available /Lindgren et al, 2002/. The model conceptualises the transport domain as a one-dimensional streamtube, which may be taken as a streamtube defined by a single particle trajectory, or as a large-scale “streamtube” in the continuum sense.

The processes considered include advection, dispersion, matrix diffusion and sorption, and chain decay. The input parameters are listed in Table 4-1. All transport parameters are constant, steady flow is assumed, and transverse dispersion is neglected. The transport equations are solved analytically for a unit pulse input in the Laplace domain, followed by a numerical inversion to the real domain. The resulting impulse-response function is then convoluted with the actual inlet boundary condition to obtain the flux-averaged concentration at the outlet. A fully numerical version of the model in under development.

As compared to the analytical solutions that constitute the basis for the flow-related parameters discussed above, FARF31 extends the process description by including dispersion and a matrix of finite extent. The flow-related parameters discussed above are based on the limiting conditions of no dispersion ($Pe \rightarrow \infty$) and an infinite matrix ($x_0 \rightarrow \infty$). The decay model is also more general than those usually accounted for in analytical solutions (single-component, first-order decay is readily included in the solutions in Appendix A). Furthermore, the numerical version of the code will allow spatially variable retardation parameters (spatial variability in the direction perpendicular to flow).

In the FARF31 code, the transport parameters must be constant along the streamtube, which means that heterogeneity cannot be modelled explicitly. This implies that the model should be parametrised by “effective” parameters that account for the effects of heterogeneity. The quantification of these “effective” parameters depends on the conceptualisation of transport in SA. In particular, a single FARF31 simulation may be performed for a large-scale, one-dimensional "tube", or for a streamtube corresponding to a single particle trajectory.

If the transport domain is viewed as a large-scale "tube", adequate statistical averaging is required when using the results from simulations of a set of single particle trajectories as input to FARF31. In principle, this means that the statistical properties of the characteristic parameter groups should be preserved for the whole ensemble of transport paths, see /Andersson et al, 1998b/. If, on the other hand, streamtubes that correspond to single particles are considered in FARF31, characteristic parameters for the individual particles should be used as input.

Single-particle streamtubes will be the main alternative for the planned SA simulations. Referring to the characteristic parameters defined above, this means that the following conditions should be fulfilled:

- Dispersion should be "small" (for the characteristic parameters to be valid). The assignment of "small" dispersivities will be based on experience and a few comparisons with results from numerical simulations using the numerical version of FARF31.
- If hydrodynamic parameters are spatially variable and retardation parameters constant, the assigned values of t_w and F should be their integrated values for each individual particle trajectory.
- If hydrodynamic and retardation parameters are spatially variable, the parametrisation should include t_w and the integrated product of F and the "material properties group" ($\sum M_i F_i$, with $M_i = \sqrt{\theta_{m,i} D_{e,i} R_i}$ in FARF31 notation, cf. Equation 4-3) for each particle trajectory.

Table 4-1. FARF31 input parameters (modified from /Lindgren et al, 2002/).

Parameter	Notation in the present report
Groundwater travel time	t_w [T]
Peclet number (quantifies dispersion)	Pe [–]
F-parameter[1]	F [TL^{-1}]
Effective matrix diffusivity of radionuclide *i*	$D_{e,i}$ [L^{2}T^{-1}]
Distribution coefficient of radionuclide *i*	$K_{d,i}$ [L^{3}M^{-1}]
Matrix porosity	θ_m [–]
Maximum penetration depth in the matrix	x_0 [L]
Decay constant for radionuclide *i*	λ_i [T^{-1}]
Bulk density of the rock (2700 kg/m^3 is assigned in the code)	ρ [ML^{-3}]
Retardation factor for radionuclide *i* in the matrix	$R_i = \theta_m + K_d \rho$ [–]

[1] In the original version of FARF31, the flow-wetted surface per volume water, a_w, was used as an input parameter. Recently, the input routine was changed to input of F. However, $a_w = F / t_w$ is calculated and used internally by the code.

It follows that the modellers should deliver particle-tracking results for all individual particle trajectories to SA.

4.6 Transport parameters in site descriptive models

4.6.1 Parametrisation of geological units

In the site descriptive modelling, primary transport data (diffusion and sorption parameters) from laboratory and in situ measurements is evaluated with the aim to develop a retardation model. This model describes the typical rock units, fractures and fracture zones within the model volume, in terms of the geometrical (different layers, etc) and retardation (parameter values) properties. Specifically, the structures are described in terms of the stratification of the altered rock, from the fracture to the unaltered (intact) rock, as well as fracture filling materials, if present.

The three-dimensional modelling of the retardation parameters implies that different rock units and "type structures" described in the retardation model are associated with (assigned to) the geological units in the descriptive geological models of the site. This means that deterministic and stochastic fractures are described in terms of the identified type structures, such that a given deterministic structure or the fractures within a given rock unit are associated with a single type structure or a combination of type structures. Similarly, the retardation properties of the intact rock within a rock unit are to be associated with rock units in the retardation model. The modelling procedure is described in Chapter 7.

Irrespective of whether the description concerns a rock unit, a fracture, or a fracture zone, the retardation parameters are the same, see Table 4-2. However, for the individual layers that make up the type structures also a typical thickness is also given. Regarding the spatial representations of the different parameters, it should be noted that the type structures present constant values of the retardation parameters of the different layers (with uncertainty intervals). The parameter for surface sorption, K_A, is not specified as a "basic deliverable" in the descriptive model, although it will be used in evaluations of sorption experiments and hence be included in the reporting of the data evaluation.

Table 4-2. Basic retardation parameters assigned to geological units.

Parameters, notation [dimensions]	Spatial representation	Comment
Effective diffusivity, D_e [L^2T^{-1}] Sorption distribution coefficient, K_d [L^3M^{-1}] Porosity, θ_m [–]	Constant or stochastic distributions for intact rock within rock units and within deterministic structures. Constant, or deterministic or stochastic assignment of parameter values to fractures within rock unit.	Retardation model describes micro-scale variability. Correlations to geometric or hydro-geological properties can be used in parametrisation of fractures.

4.6.2 Parametrisation of flow paths

The parametrisation of flow paths with flow-related transport parameters is based on simulations of flow paths in groundwater flow models. As described in Section 4.2, the flow-related parameters can be calculated directly in the groundwater flow models, which could require additional parametrisation (geometric and/or retardation parameters) compared to the purely hydrogeological analyses, and/or in separate models using the results of flow path modelling as input. The geometric framework for these parameters, that is, the pathways for solute transport, is defined by the flow field and the transport boundary conditions (the injection locations), and is therefore not directly related to the units/domains in the geological model. Thus, the flow-related parameters will be presented in reports, not in the framework of the RVS model.

The flow-related transport parameters are summarised in Table 4-3. Note that the table is focused on the main parameters to be evaluated and reported. In cases where the retardation parameters are spatially variable, other parameters, primarily the “total transport resistance” (Equation 4-3) and the “surface sorption parameter group” (Equation 4-2), will be calculated (see Section 4.3.3). The aim is to obtain a stochastic description of the flow-related parameters. It should be noted that randomness is due to different factors, e.g. the stochastic description of flow and uncertainties related to alternative injection locations, which means that the specification of relevant performance measures is important.

For the Safety Assessment calculations, also the Darcy fluxes at the release locations for particles should be reported. It should be noted that the distributions of flow-related parameters depend on the release locations, and that SA and the site descriptive modelling will consider different sets of release locations. As described in Section 7.2, the simulations that produce the flow-related parameters should be specified in Task Descriptions to the groundwater flow modellers (see also /Rhén et al, 2003/).

Table 4-3. Flow-related transport parameters.

Parameters, notation [dimensions]	Spatial representation	Comment
Travel time, t_w [T]	Stochastic distributions	Calculated using ground-water flow models. Geometric[1] and retardation parameters can be given as input to flow models or be handled separately.
“F, F [TL^{-1}]	Stochastic distributions	
Materials parameter group, $M = \sqrt{\theta_m D_e R_m}$ [LT$^{-1/2}$]	Constant or stochastic distributions	

[1] For example, the “effective width” of flow paths, see text.

4.7 Transport modelling in other disciplines

Transport modelling will be performed as a part of site descriptive modelling within other disciplines. In particular, transport parameters are required for the modelling of density-dependent groundwater flow in Hydrogeology. Different parameters are needed in different modelling approaches. Specifically, two main modelling approaches can be distinguished:

- The classical continuum-based approach, in which advective-dispersive transport of salt is modelled without interactions between mobile and immobile zones. In this approach, different porosities are often used for flow and transport, such that the observed “retardation” of solute transport can be taken into account. Thus, different “effective” porosities for flow and transport may be required. In addition, dispersion parameters are required.
- Modelling approaches that consider mass transfer between mobile and immobile zones. Density-dependent flow and salt transport influenced by mass transfer can be modelled with the DarcyTools code, which will be used during the Site Investigations (Section 3.3.3). In DarcyTools, multiple mass transfer domains can be considered by a “multi-rate approach”. Distributions of rates and “capacities” of the immobile zones are required as inputs (cf. Section 4.3.2). In addition, dispersion within the mobile zone may be taken into account, although most simulations likely will be performed without any dispersion.

It should be noted that dispersion is scale-dependent, and that the relevant scale for salt transport may differ from that/those considered in radionuclide transport. In practise, the modelled dispersion may in many cases be determined by the grid scale-dependent numerical dispersion.

Rather than providing a detailed description of the transport parameters that may be required, we emphasise at this stage the need for interactions between Hydrogeology and Transport regarding transport parameters for salt. Specifically, these interactions should take place in connection with the development of Task Descriptions (Section 7.2) for the groundwater flow modelling. It should be noted that the assignment of parameters for salt transport to large extent will be based on experiences from previous modelling efforts, and that very little site-specific data that can support these parametrisations is produced within the Transport programme. However, different types of tracer tests could provide data for this purpose. Also, comparisons between measured and modelled salinity distributions could provide a means to assess the parameters used for salt transport calculations.

Similarly, the transport parameters that may be needed within other disciplines, primarily Hydrogeochemistry, are not specified here. In principle, both advective-dispersive and travel time-based approaches can be taken, which would require different sets of input parameters. The implications of possible differences in scales that are mentioned above apply to the hydrogeochemical transport simulations as well.

4.8 Methodological inputs

As mentioned in Chapter 2, the present strategy is to large extent based on experiences from the TRUE project and other research at Äspö HRL. This influence concerns both the strategy for laboratory measurements /Widestrand et al, 2003/ and the present strategy for site descriptive modelling. In particular, the main methodological inputs to the modelling strategy are:

- The methodology for parametrisation of structures that was developed by the Äspö Task Force, Task 6C /Dershowitz et al, 2003/.
- The methodology for parametrisation of flow paths that was developed during the TRUE project /Poteri et al, 2002; Cvetkovic and Cheng, 2002/.

Other relevant references are listed in Section 2.11. In particular, the TRUE project has contributed also with conceptual models and characterisation data related to sorption and diffusion processes. In addition, important experience regarding flow-related transport parameters was gathered during the Alternative Models Project, a subtask of SR 97 /Widén and Walker, 1999; Gylling et al, 1999; Dershowitz et al, 1999; Selroos et al, 2002/. It should also be noted that the treatment of spatial variability along flow paths is consistent with the approach proposed by /Andersson et al, 1998/.

In the SR 97 project, the transport calculations were based on the Stochastic Continuum code HYDRASTAR. Flow-related transport parameters were calculated from Darcy fluxes using uniform (constant in space) values of the effective (flow) porosity and the "flow-wetted surface". The main differences between the transport modelling within SR 97 and the modelling to be carried out during the Site Investigations are:

- DFN-based groundwater flow models will be used as the main tools for particle tracking simulations. This means that the required geometric parameters can be calculated in the models, based on the geometric description of the fracture network.
- Spatial variability in sorption and diffusion parameters will be considered. The emphasis is on longitudinal (along the flow paths) variability; however, also transverse (into the matrix) variability will be addressed.

4.8.1 The Task 6C methodology

This section summarises the Task 6C methodology. The aim is to illustrate the main components of the analysis, since these are similar to the basic steps in the strategy proposed in the present report. However, this is not to say that exactly the same methodology will be followed in the site descriptive modelling. For example, the number of type structures will be site specific, and other parameters may be found more appropriate for characterising the heterogeneity of the larger structures. It is foreseen that the experiences from the ongoing work within Task 6C will be important for further development of the present strategy.

Figure 4-2 illustrates the procedure for parametrisation of structures with retardation parameters that was developed within Task 6C /Dershowitz et al, 2003/. The methodology is based on an identification and parametrisation of "type structures". Two such "type structures" were defined, referred to as micro-structural models/elements Type 1 and Type 2.

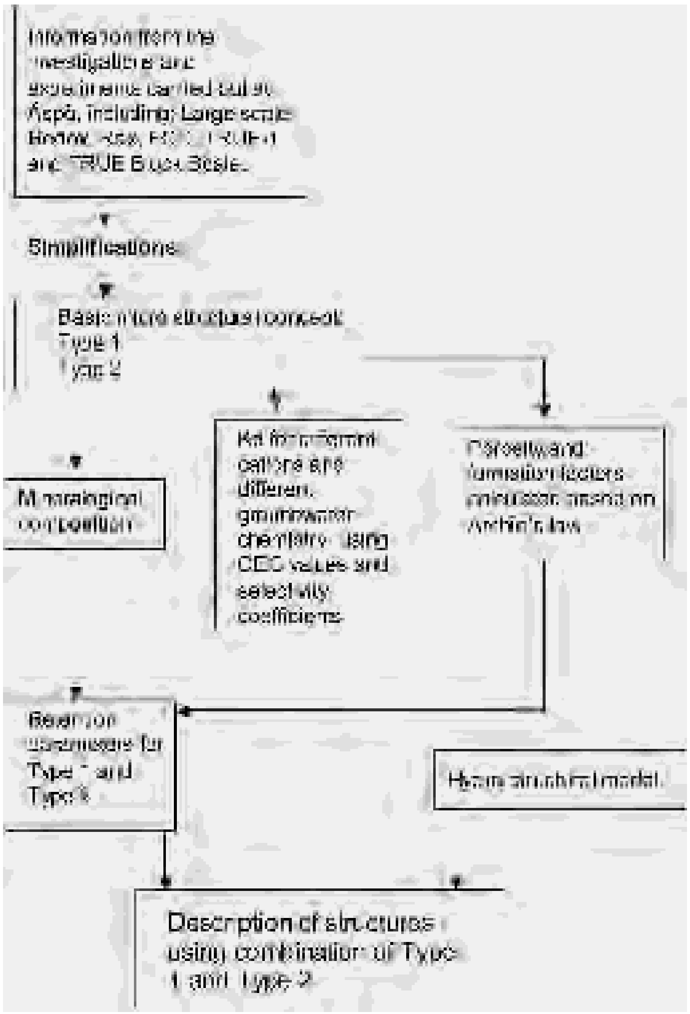


***Figure 4-2.** Flow chart showing the procedure for parametrisation of structures with retardation parameters in Task 6C /from Dershowitz et al, 2003/.*

The structures in the hydro-structural model were then parametrised using the type structures, either with individual type structures (for small structures) or with combinations of the two type structures (larger structures). In the present context, the micro-structural models would correspond to the retardation model (Chapter 6), and the hydro-structural model to the hydrogeological site descriptive model.

It is important to note that the parametrisation to a large extent relied on interpretations and "expert judgement" of what could be regarded as "typical" structures and materials, rather than on direct evaluations of spatial variability from geometrically oriented "point samples" at the site. Specifically, the interpretations were based on an identification of basic structure types, the different material layers that make up these structures, and how the basic structures combine to form larger structures.

The main advantage of the Task 6C methodology is that, once the "typical" structures and the materials they "typically" consist of have been identified and adequately described, the sorption and retardation parameters for a particular material/layer can be obtained from any sample that complies with the description. Thus, the description of spatial variability involves elements of classification that simplify the description and reduce the number of samples required to characterise the variability. A parametrisation that strictly honours parameter values only where they are sampled would require a much larger number of samples. Furthermore, any alternative description that does not focus on the intact rock only (long term perspective) must use the geometric structure provided by the flow paths as a starting point.

The main simplifications in the Task 6C approach are shown in Figure 4-3. It can be seen that the DFN description was used as a basis for the parametrisation. In particular, the fracture size (length) had a key role, since both hydraulic and retardation parameters were assigned to the individual structures based on correlations to the size. Thus, the assignment of basic micro-structural model Type 1 or Type 2 to the structures was stochastic. Furthermore, a “complexity” parameter was used to express how the basic models should be combined to “construct” the structures. This parameter is primarily relevant for the larger structures.

Thus, the methodology proposed in Task 6C assigns “type structures” and their associated retardation parameters to the individual structures in a DFN description. Calculations of flow-related parameters are straightforward if performed directly in the DFN model. However, additional developments are required for applications involving “mixed” DFN/SC codes such as DarcyTools. In particular, the treatment of the retardation parameters when transforming the DFN description to a continuum requires further development.

The Task 6C methodology is considered to be a suitable framework for the descriptive modelling during the Site Investigations. Therefore, it is proposed that the parametrisation should be performed according to the principles outlined above, and that the aim is to develop a similar description as that of the “semi-synthetic” structures in Task 6C. However, it is also foreseen that simplified approaches need to be taken at the early SI stages, and that the methodology needs to be further developed. For example, other parameters than the fracture size may be found more appropriate for developing correlations, and the use of the “complexity” parameter in the parametrisation of structures should be evaluated. As indicated above, the use of other flow modelling approaches implies that developments are required.

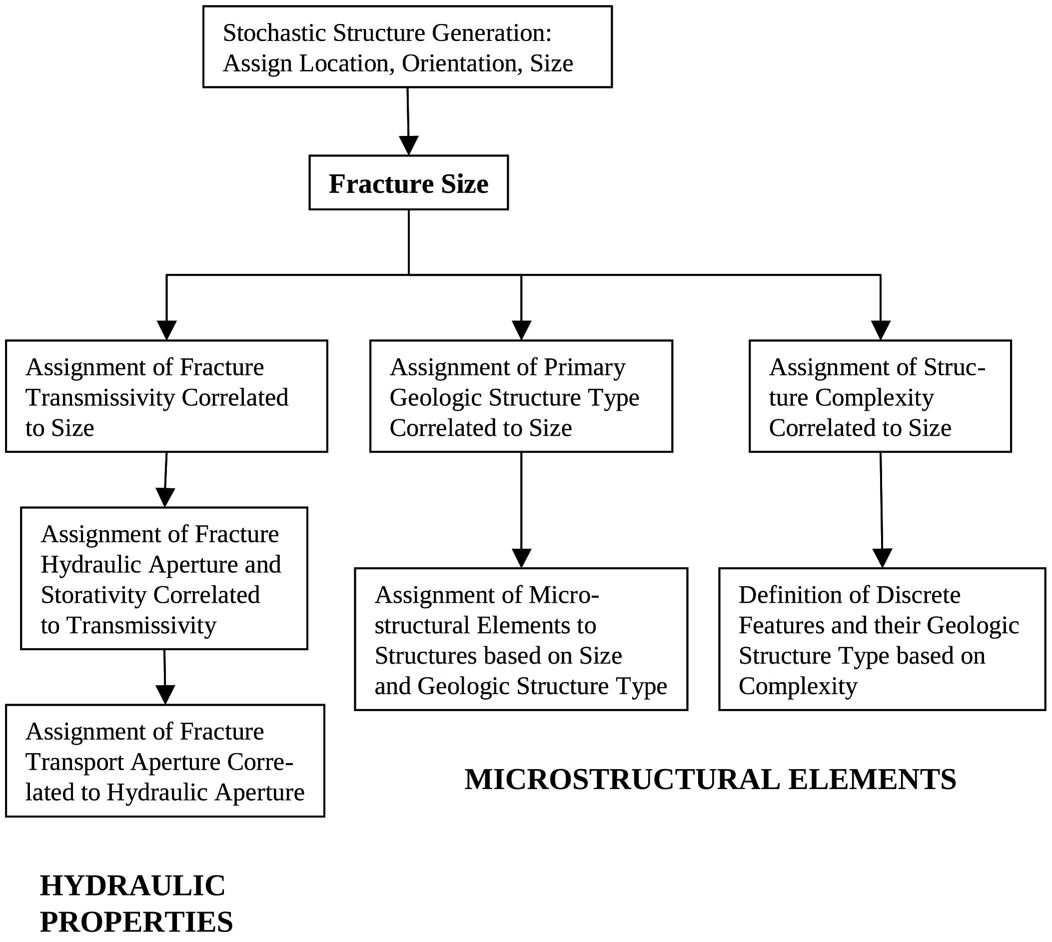


Figure 4-3. *The main simplifications involved in the Task 6C parametrisation /from Dershowitz et al, 2003/.*

4.8.2 Inputs from the TRUE programme

As discussed above, the TRUE programme, especially the TRUE Block Scale project, is an important source to process understanding and a basis for model development. The main methodology-related inputs from TRUE Block Scale to the transport properties modelling can be summarised as follows /Poteri et al, 2002; Cvetkovic and Cheng, 2002/:

- A theoretical basis for the quantification of combined advection and retardation variability along flow paths (see Appendix A).
- A methodology for quantitative, statistical analysis of the (hydrodynamic) transport resistance. In particular, model/parameter simplifications (in view of the statistical description) were assessed, and useful methods and tools for this analysis were presented.
- A methodology for modelling transverse (into the rock matrix) spatial variability was developed.
- Modelling was performed with a number of different codes, which demonstrated the capabilities of different models and modelling approaches, as well as the benefits of a “multi-model approach”.

In particular, the following methods for estimating the transport resistance were applied and compared (specifically, the analysis was focused the parameter $k \equiv F / t_w$):

- Numerical Monte Carlo simulations in DFN models (k was obtained through linear regression of F and t_w).
- Estimates based on a streamtube model, where the width of the streamtube was estimated as the diameter of the injection borehole (the analysis concerns tracer test evaluations).
- Estimates based on an interpreted inverse half-aperture (see equations in Appendix A).

This should not be understood such that exactly the same modelling approach will be taken during the Site Investigations. However, in the TRUE Block Scale tracer test evaluation reported by /Cvetkovic and Cheng, 2002/, DFN simulations were used as the main tool for quantifying flow-related parameters and investigating model simplifications, whereas other, simplified methods (cf. above) were used for comparative purposes. This strategy will be used also in the site descriptive modelling.

Concerning the TRUE-1 experiment, it should be noted that different interpretations of the results have been made. Specifically, the experiment has not resolved whether the apparent retention that was observed in tracer tests could be attributed to (1) fracture/rock matrix interactions in a single fracture /Cvetkovic et al, 2000/, (2) multiple pathways with retention occurring in fine-grained gouge material /Mazurek et al, 2002; Jacob et al, 2002/, or (3) three-dimensional flow effects (increased surface area for mass transfer; /Neretnieks, 2002/. However, it should be noted that the basic mechanisms considered in the different evaluations of the experiment were the same, and also the same as in the main modelling approach proposed in the present strategy.

4.9 Tools for analysis, interpretation and modelling

In the process of developing Site Descriptive Models, the Transport programme uses evaluation and modelling tools for the following main purposes:

- *Descriptive modelling:* RVS (Rock Visualisation System) will be used for descriptive modelling of retardation parameters. RVS modelling is described by /Munier et al, 2003/.
- *Evaluation of laboratory and field measurements:* Primary data are in many cases obtained by calculating parameter values from, e.g. measured concentrations. The tools used for this purpose range from analytical solutions (e.g. solutions to diffusion equations) to numerical transport codes used in the evaluation of tracer tests.
- *Calculations of transport parameters in site descriptive models:* Groundwater flow models and transport codes will be used for determining the parameter values to be assigned to geological units and flow paths. In addition to the needs directly associated with parametrisation, model calculations will be an important component in the development of a geoscientific understanding of the investigated sites.

The transport codes that were used within the TRUE Block Scale project represent a recent compilation of modelling approaches and available tools. As an illustration of the capabilities of existing models, these codes are summarised in Table 4-4. For a more detailed account of the various models it is referred to /Poteri et al, 2002/.

It is foreseen that some of the codes listed in Table 4-4 will be used also during the Site Investigations, primarily for analysing tracer tests (especially the codes referred to as SKB-WRE and SKB-GEOSIGMA). In addition to the models in the table, the Safety Assessment transport code FARF31 (see Section 4.5) and transport models/routines connected to the groundwater flow models DarcyTools and CONNECTFLOW will be used. Furthermore, other previously applied codes, such as the channel network code CHAN3D /Gylling et al, 1999/, can be employed in the transport modelling. Finally, transport models that include a more general set of hydrogeochemical processes (e.g. LaSAR-PHREEQC; /Malmström et al, 2004/) may also be considered in studies of alternative/complementary retention models.

Table 4-4. Transport models used in the TRUE Block Scale project /Poteri et al, 2002/.

Modelling group/model	**Modelling approach**	**Representation of flow domain**	**Transport processes**[1]
ENRESA-UPV/UPC	Stochastic Continuum	Multiple 3-D elements	3-D Advection Dispersion (L,T)[2] 1-D Matrix diffusion and sorption[3]
Nirex-Serco	Discrete Fracture Network	Multiple interconnected 2-D elements (open fractures, unit porosity)	2-D Advection Dispersion (L) 1-D Matrix diffusion and sorption
JNC-Golder	Channel Network	Multiple interconnected 1-D elements (open fractures, unit porosity)	1-D Advection Dispersion (L) 1-D Matrix diffusion and sorption
Posiva-VTT	Streamtube	Non-connected 1-D paths	1-D Advection[4] Dispersion[5] 1-D Matrix diffusion and sorption with multiple retention zones
SKB-WRE	LaSAR (Lagrangian Stochastic Advective Reactive)	Non-connected 1-D paths	1-D Advection[4] 1-D Matrix diffusion and sorption with spatially variable properties in the direction of diffusion
SKB-GEOSIGMA	1-D Advection- Dispersion	1-D constant velocity	1-D Advection Dispersion (L) 1-D Matrix diffusion and sorption

[1] Dimensionality of advection refers to the "basic units" in the description; advection in models with 1-D and 2-D "basic units" (e.g. interconnected "pipes") may be 3-D on the field scale.
[2] L = longitudinal, T = transverse
[3] Not modelled explicitly in the 3-D model
[4] Travel time distributions for "collections" of paths
[5] By "correction" of the travel time distribution

5 Identification and acquisition of data

During the Site Investigations, the Transport programme will conduct laboratory and field measurements resulting in the Primary Data that constitute the main discipline-specific inputs to the Transport Properties Site Descriptive Modelling. Although not strictly a modelling activity, the data collection is for obvious reasons important for modelling. Interactions are necessary in the planning of sampling and analyses, and a timely access to data is critical for the progress of modelling. In particular, updates of the measurement programme may be necessary in view of the analyses of uncertainty and confidence performed by the modelling projects.

The strategy for planning and execution of laboratory measurements is presented by /Widestrand et al, 2003/. In this chapter, we summarise some key points of the laboratory strategy, and give modelling-related guidelines for the implementation. In particular, the characterisation methods and the control of the sampling and analysis programme are summarised.

5.1 Characterisation methods

5.1.1 Laboratory methods

Method Descriptions (MD) have been developed for the two main characterisation methods within the Transport programme:

- *Through-diffusion measurements* (MD 540.001), which are used primarily for determining the effective diffusivity, D_e, of geological materials. Specifically, the Method Description is focused on measurements of D_e for non-sorbing tracers.
- *Batch sorption measurements* (MD 540.002), which are used primarily for determining volumetric distribution coefficients, K_d, for different radionuclides in different systems of geological materials and (ground)waters.

Through-diffusion and batch sorption measurements are the main methods for obtaining site-specific data on diffusion and sorption parameters, respectively, during the Site Investigations. However, also other laboratory methods will be used. These methods include less resource-demanding methods that are used to assess spatial variability, and methods used in the process of selecting samples for detailed measurements.

Through-diffusion measurements

Through-diffusion measurements are carried out by measuring the diffusive transport of a tracer through a rock sample. The sample is placed in a diffusion cell, where it is saturated with a solution of known chemical composition. A solution containing the tracer is applied in a “reservoir” at one end of the sample and the increase in tracer concentration in the initially tracer-free “reservoir” at the other end is measured. The concentration breakthrough curve is then evaluated to obtain a value of the effective diffusion coefficient, D_e. Both non-sorbing and sorbing tracers can be used. In the latter case, also the distribution coefficient, K_d, can be evaluated. The tracer selection is a critical component of the experimental design, especially since experiments with strongly sorbing tracers are highly time-consuming.

The strategy for the through-diffusion measurements during the Site Investigations is to determine D_e for tritiated water (HTO), and then use tabulated values of the diffusivity in water, D_w, to calculate rock type specific values of the formation factor, $F_m = D_e / D_w$ (see Section 4.3.2). This formation factor can then be used to calculate the effective diffusivities of other solutes in that particular rock type, provided that their diffusivities in water are known.

It follows that HTO is to be used as the main reference tracer in the determination of effective diffusivities. However, it is also proposed to perform a small number of diffusion experiments with sorbing tracers (preferentially Cs^+ and Sr^{2+}), primarily for addressing the observed inconsistency between the K_d values obtained in diffusion experiments and those evaluated from batch sorption tests. For Cs^+, it is unlikely that breakthrough curves will be obtained within a realistic time frame. Penetration profile studies will therefore be necessary for that tracer.

Detailed method-specific recommendations for the through-diffusion measurements are given by /Widestrand et al, 2003/. These recommendations cover important factors such as the selection of water for saturation of the samples (based on identified typical water compositions at the sites), the selection of sample length(s), the use of rock sample replicates to investigate micro-scale spatial variability, and the handling of differences in stress state.

Other laboratory methods for diffusion measurements

Through-diffusion measurements are highly time-consuming, and hence there is a need for other, complementary methods that can be applied for addressing spatial variability by measurements on a larger number of samples. Laboratory resistivity measurements is the main method to be used for this purpose during the Site Investigations. This method is also used within the Geology programme, and a MD has been developed by Geology (MD 230.001). Since the experimental procedure described in the MD deviates from previous (and planned) measurements in studies of transport properties, a comparative study has been initiated. This study may lead to a revision of the MD, which makes it possible to use the same method in both disciplines. Also gas diffusion measurements are planned, but these will likely be limited to a few samples only. At present, no MD is planned for these measurements.

In laboratory resistivity measurements, the rock sample is saturated with an electrolyte of known composition and properties. Resistivities are measured on the sample and on the pure electrolyte, and the formation factor of the rock is evaluated from the relation of the resistivity values. Resistivity measurements will be performed on a relatively large number of samples /see Widestrand et al, 2003/. The calibration of the method is important for the use of the results. This is done by direct comparison with through-diffusion measurements on identical samples. Furthermore, to enable comparisons between the methods the same sample lengths should be selected.

Batch sorption measurements

Batch sorption measurements are performed by measuring the sorption of a tracer on crushed rock material in a measurement cell initially containing the rock material and the tracer dissolved in water of known composition. The decrease in dissolved concentration is measured as a function of time, and sorption coefficients are evaluated based on the concentrations measured after certain contact times; these contact times are specified in the MD. Sorption coefficients can be evaluated using non-linear or linear sorption models. In the Site Investigations, the modelling is based on the assumption of linear sorption (see Chapter 4).

A general measurement programme, where a number of concentration measurements are to be performed on all sampled geological materials in all water types considered relevant and for a large number of tracers, soon becomes unrealistically resource demanding. Therefore, a procedure based on different characterisation levels for different tracers is proposed, see Table 5-1. This procedure is based on a hierarchic principle where a majority of the samples (75%) are investigated with a scanning method (determination of CEC, Cation Exchange Capacity) only. This method does not provide sorption parameters directly, but these can be inferred from databases in cases where CEC is judged not to deviate from what can be expected for that particular rock type (see /Widestrand et al, 2003/ for a detailed discussion).

For the remaining samples (25%), experimental determination of sorption coefficients will be performed. However, since a "complete" programme even for this reduced amount of samples would be very large, a ranking is performed in order to select the combinations of tracers, geological materials and water types that are judged to be the most important for Safety Assessment. An iterative process is foreseen, where Safety Assessment provides feedbacks that guide further laboratory measurements. In the strategy proposed by /Widestrand et al, 2003/, a site specific database for K_d-values is developed by measurements according to the levels A–C and comparisons with existing databases.

The selection of size fractions of the geological materials in the batch sorption experiments is a factor that can affect the results. Essentially, there is some evidence that sorption coefficients, at least under some conditions, may depend on the size fraction investigated. Therefore, gas adsorption measurements (BET measurements) will be used to quantify active surface areas, and different experimental approaches will be taken depending on the outcome of these measurements.

Table 5-1. Selections of radionuclides within the different levels of batch sorption experiments.

Level	Selection type	Procedure/radionuclides
C	Determination of cation exchange capacity (CEC) combined with specific surface area BET measurement	Procedure according to ISO 13536 (CEC) and ISO 9277:1995 (BET)
B	Level C + Sorption experiment using Cs^+, Sr^{2+} and Am(III)	$^{134}Cs^+$, $^{85}Sr^{2+}$, ^{241}Am(III)[1]
A	Level B + Selection of radionuclides/elements representing different oxidation states, safety assessment perspective	$^{134}Cs^+$, $^{85}Sr^{2+}$, $^{226}Ra^{2+}$, $^{63}Ni^{2+}$, ^{241}Am(III)[A], ^{234}Th(IV), $^{99}Tc(VII)O_4^-$, $^{233}U(VI)O_2^{2+}$, $^{237}Np(V)O_2^+$
in situ experiment tracers	Weakly and moderately sorbing tracers, possible use in in situ experiments	$^{22}Na^+$,$^{45}Ca^{2+}$, $^{83}Rb^+$, $^{85}Sr^{2+}$, $^{134}Cs^+$, $^{133}Ba^{2+}$, $^{54}Mn^{2+}$, $^{57}Co^{2+}$

[1] Lanthanide isotopes can be used instead of ^{241}Am, see /Widestrand et al, 2003/.

Porosity measurements

Porosity measurements will be performed using both water saturation and PMMA techniques. The PMMA method, in which slices of rock samples are impregnated with a monomer of low viscosity, is described in a separate MD (MD 540.003). Porosity measurements by the water saturation method are included in the MD for through-diffusion measurements (MD 540.001). Specific recommendations for these measurements are given by /Widestrand et al, 2003/.

5.1.2 In situ (field) methods

Laboratory measurements are the main source of discipline-specific Primary Data. However, also in situ measurements will be performed. With regard to the in situ methods, we can make a distinction between two different types of methods:

1. Methods that provide information on parameters that are also measured in the laboratory programme (retardation parameters).
2. Methods that provide information on other parameters (primarily parameters related to flow and advection).

In situ measurements of retardation parameters

The in situ methods for measuring (primarily) retardation parameters include:

- In situ resistivity logging (formation factor logging)
- In situ tracer borehole sorption/diffusion experiments
- Single-Well Injection-Withdrawal tests (SWIW)

These methods can provide information on spatial variability and scale dependence of retardation parameters, which are important factors for parametrisation and assessment of uncertainty and confidence. In particular, the aim of the **resistivity/formation factor logging** is to obtain a profile of the formation factor (which can be used to calculate the effective diffusivity) along the investigated borehole, see /Löfgren and Neretnieks, 2002/.

Similar to the laboratory resistivity measurements (Section 5.1.1), the resistivity of the pore water must be known when calculating the formation factor of the rock. Since the "samples" are not accessible and thus cannot be saturated with a known fluid, this requires measurements of the resistivity of the rock pore water along the borehole. Furthermore, groundwater flow from fractures cause disturbances that must be removed in the interpretation of the in situ results.

In situ borehole sorption/diffusion measurements have been suggested as a method for measuring the sorption and diffusion properties of the rock matrix under field conditions. In this method, a solution containing sorbing and non-sorbing tracers is circulated in a packed-off section of "fracture-free" rock in a borehole. Thus, the intention is to find "fracture-free" rock matrix and characterise its diffusion and sorption properties in situ. The circulation is performed to obtain a homogeneous solution within the section, and to enable measurements of tracer concentrations. The retardation parameters of the rock matrix are then evaluated from the measured concentration decline in the investigated section.

Whereas the in situ sorption/diffusion method is targeted on "fracture-free" rock along boreholes, **single-well injection-withdrawal (SWIW) tests** have been proposed as a method for investigating the transport properties of conductive features that intersect boreholes /Nordqvist and Gustafsson, 2002/. Essentially, SWIW tests are carried out by injecting a tracer pulse containing tracers of different sorption properties, possibly followed by injection of a "chaser" fluid to push the tracers further away from the borehole. After a "resting period", during which mass transfer and sorption/diffusion in the immobile zones may occur, pumping is reversed and the (remaining) solution is pumped back to the borehole. Advection and retardation parameters are then quantified by evaluation of measured concentrations, using analytical or numerical transport models.

The in situ methods have the advantage of measuring the various transport parameters under realistic field conditions in terms of the geological and hydrogeochemical environment, and, in many cases, also the scales at which the processes are studied. In addition, the in situ methods incorporate the natural spatial variability, either by providing spatial distributions (e.g. resistivity logging) or in an integrated/average sense (e.g. tracer tests). However, the fact that the measurements are carried out in situ also makes the interpretation of the results more difficult than under well-controlled conditions in the laboratory.

The in situ methods discussed above are still under development, and it is therefore uncertain to what extent they will contribute in the process of data gathering and site descriptive modelling. Methodology tests will be conducted during the Initial Site Investigation phase. The potential for contributions from in situ measurements of retardation parameters can be judged when these tests have been evaluated.

Other in situ methods

The in situ methods for measuring (primarily) advection parameters include:

- Multi-Well Tracer Tests (MWTT)
- Groundwater flow measurements

Multi-well tracer tests (MWTT; MD 530.006) and SWIW tests have several common features and can, in principle, both be used to quantify advection and retardation parameters. It is foreseen that essentially the same tracers will be used, non-sorbing tracer and weakly sorbing tracers as listed in Table 5-1, in applications of these two methods. In the present context, however, we consider SWIW primarily as a method for obtaining retardation parameters, whereas MWTT is regarded mainly as a method for investigating flow patterns and advective transport. Clearly, this general guideline should be implemented with flexibility, especially since the usefulness of SWIW tests has yet to be evaluated.

MWTT with both sorbing and non-sorbing tracers have been used in many research projects, e.g. the TRUE experiments at Äspö HRL. However, during the Site Investigations the main use of MWTT will be as a method for testing the confidence in the hydrogeological model, that is, to investigate the connectivity of the fracture network. In addition, tracer tests may be performed in order to investigate specific geological structures, and to determine advection parameters (e.g. effective porosities and dispersivities) at scales relevant for different types of transport models.

The Transport programme also includes **groundwater flow measurements**. These measurements are performed as dilution tests in packed-off sections along boreholes. This means that a tracer-containing solution is circulated within the investigated section, and that the decrease in tracer concentration(s) that takes place due to through-flow of groundwater is measured as a function of time. The flow rate is then quantified based on curve fitting with an analytical solution. Theory and evaluation methods for dilution tests are described by /Andersson et al, 2002d/.

Groundwater flow measurements by dilution techniques can be performed with different types of equipment, ranging from measurements within sections between fixed packers to special probes that can be moved along the borehole. Table 2-1 refers to a specific method for groundwater flow measurements (MD 350.001), in which the “dilution probe”, described by /Gustafsson, 2002/, is used. This equipment can also be used for SWIW tests, such that SWIW tests are preceded by flow measurements that provide input data for the design of the tracer tests. Other methods for groundwater flow measurements are handled by Hydrogeology.

5.2 Methodology and controlling documents

The sampling of geological materials from drill cores and the laboratory measurements are controlled by the Sampling and analysis plan. This plan is developed through a sampling and method requirement analysis that requires input from the models developed by Geology, Hydrogeology and Hydrogeochemistry. The process is illustrated in Figure 5-1. As indicated in the figure, the Sampling and analysis plan should reflect a number of different interests and goals. It is foreseen that planning meetings with representatives for the different disciplines that produce models and/or sample drill cores will be an important component in the development of the plan.

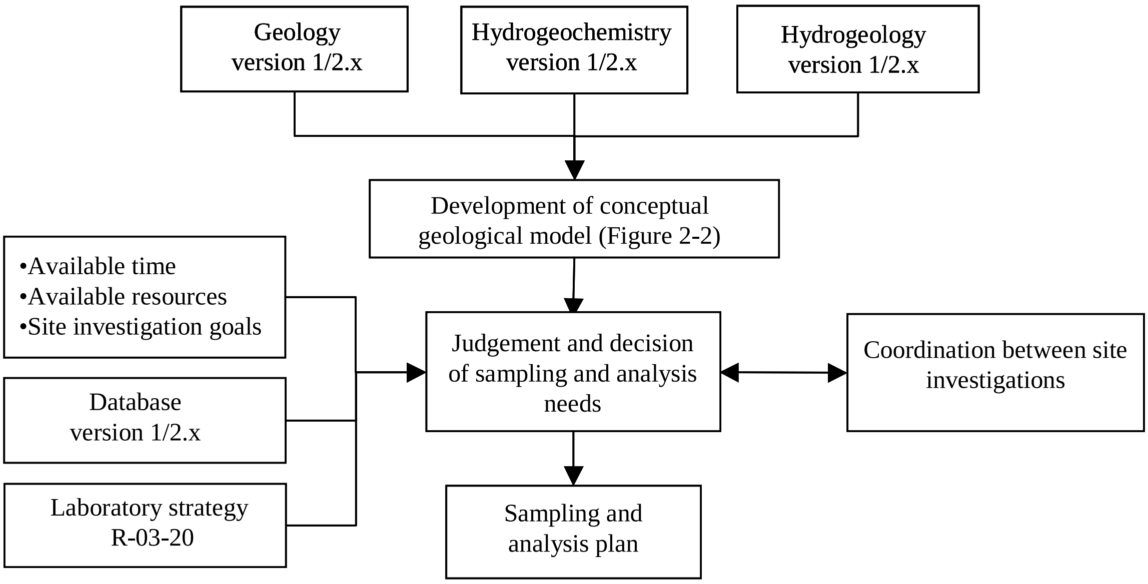


Figure 5-1. *Flow chart for the decision of sampling and analysis needs (from /Widestrand et al, 2003/; the figure number refers to their report).*

5.3 Contents of the retardation database

Sampling of drill cores is registered in SICADA (SIte ChAracterisation DAtabase) in accordance with SKB routines. All data entries in SICADA have a geographic reference, which means that it is linked to a point on the surface, or along a tunnel or a borehole. The site-specific retardation databases that are developed during the Site Investigations should contain all the measured data, but measured data only. This means that measured screening parameters should be included, whereas parameters interpreted based on these screening parameters should not. For example, measured CEC values are to be included in the database, but not the K_d values interpreted from these CEC values. The data is inserted in fields in the database that are linked to the unique sample identification number.

Additional data on the preparation of the sample, a geological description and its in situ stress state, and the analyses performed, are also valuable to add to the database. Each of these fields are then linked to the sample ID. /Widestrand et al, 2003/ provide a hypothetical example of an extended database sheet that contains detailed sampling and sample characterisation data.

5.4 Modelling-related guidelines

Sampling and analysis, and the Primary Data that results from these activities, is the basis for the site descriptive modelling. Hence, the outcome of the modelling, especially the uncertainties and the possibilities of describing spatial variability, is to large extent determined already at the sampling stage. Below, a few guidelines of importance for the modelling are given.

- The observed inconsistencies between different laboratory methods should be addressed. Two types of inconsistencies have been observed in previous studies: (1) applications of (seemingly) the same methods have yielded different results, and (2) applications of different methods for determining the same parameter (e.g. the matrix sorption coefficient) have yielded different results. In the first case, consistency could be achieved by a rigorous definition of the experimental conditions, whereas the second type of inconsistencies requires comparisons and specific investigations of differences between methods. This implies that a data set must be available that allows such comparisons, and more detailed analyses, if necessary. These issues are considered in the proposed laboratory strategy.
- For the assessment and quantification of spatial variability, it is an advantage if different parameters are measured so that they can be taken as representative of the same "point" in the model domain. In other words, it is important that correlations between different parameters can be investigated. This means that different retardation parameter should be determined for "the same sample", and that laboratory investigations of fracture materials should be directed towards structures that have been characterised hydraulically.
- Whether a proposed characterisation level is sufficient cannot be evaluated if the goal of the characterisation effort has not been specified. Although this is to some extent a site-specific matter (it depends, for instance, on the number of geological units identified at the site), and should be discussed in connection with the development of the Sampling and analysis plan, a few general guidelines can be proposed:
    - The spatial variability in the retardation parameters of the intact rock within the main geological units should be expressed in terms of statistical distributions. Thus, sufficient data must be collected to facilitate this description.
    - For minor rock units and structures (that is, the individual layers in the description of the structures), the available data should be sufficient for identifying typical values or intervals of the retardation parameters.

6 Evaluation of primary data

The evaluation of Primary Data includes both discipline-specific activities and activities that involve several disciplines. In particular, the data evaluation within the Transport programme is strongly linked to data and models produced by Geology. We define here all activities associated with the development of the “retardation model” (see Section 2.10) as evaluation of primary data. Thus, the retardation model is regarded as the final product of the data evaluation step in the site descriptive modelling. It is also the final product of the laboratory programme described by /Widestrand et al, 2003/, who we refer to for a more detailed description of the retardation model development.

6.1 Aim and methodological inputs

According to the definition in Section 2.10, the retardation model is an interpreted description (including interpreted data) of retardation properties for the typical rock units and structures. It comprises a rock unit description, descriptions of the typical layers for fractures and fracture zones, and a database with interpreted porosity, sorption and diffusion data for the different materials.

It follows that the methodology for parametrisation of rock mass and structures with retardation parameters comprises the following basic steps:

1. An identification of the different units (rock mass and structures) that will be described as separate units in the retardation model.
2. An identification of the layers/materials that will be described for the different units.
3. A parametrisation of the layers/materials of the units with interpreted retardation parameters.

The strategy proposed here is based on the work by /Dershowitz et al, 2003/, who developed “micro-structural models” for two basic fracture types and used these models as a basis for parametrisation of fractures and fracture zones in a hydro-structural model. It is important to note that once the materials in the rock units and in the individual layers that make up the structures have been identified and adequately described (geologically and hydrogeochemically), the retardation parameters are obtained from an interpretation of the properties of that material. This means that all characterisation data for that material can be used for assigning parameter values. An alternative approach where the model is developed from strictly geometrically oriented data (as in geostatistical models for flow parameters) is, because of the many different materials and the associated sampling and analysis needs, not considered feasible in this case.

6.2 Methodology for development of the retardation model

The working methodology for development of retardation models is illustrated in Figure 6-1. The interpretation of Primary Data involves compilation and evaluation of data for different sample types defined with the aid of the geological model. Data are compared and evaluated regarding /Widestrand et al, 2003/:

- observed differences in properties between different rock types and materials,
- impact of structural/textural variations, alterations, sampling depth, etc,
- homogeneity/heterogeneity in defined rock sample types,
- extreme values or materials,
- uncertainty in data,
- differences between laboratory and field data (provided that field data is available).

The site-specific database is compared with the generic database, in order to identify deviations and to establish the level of agreement in data. For a final acceptance of the site-specific database, a general consensus in the understanding and confidence in the quality of the database is required. The retardation model is then constructed or updated in accordance with the strategy described by /Widestrand et al, 2003/. Examples of hypothetical retardation models are given below.

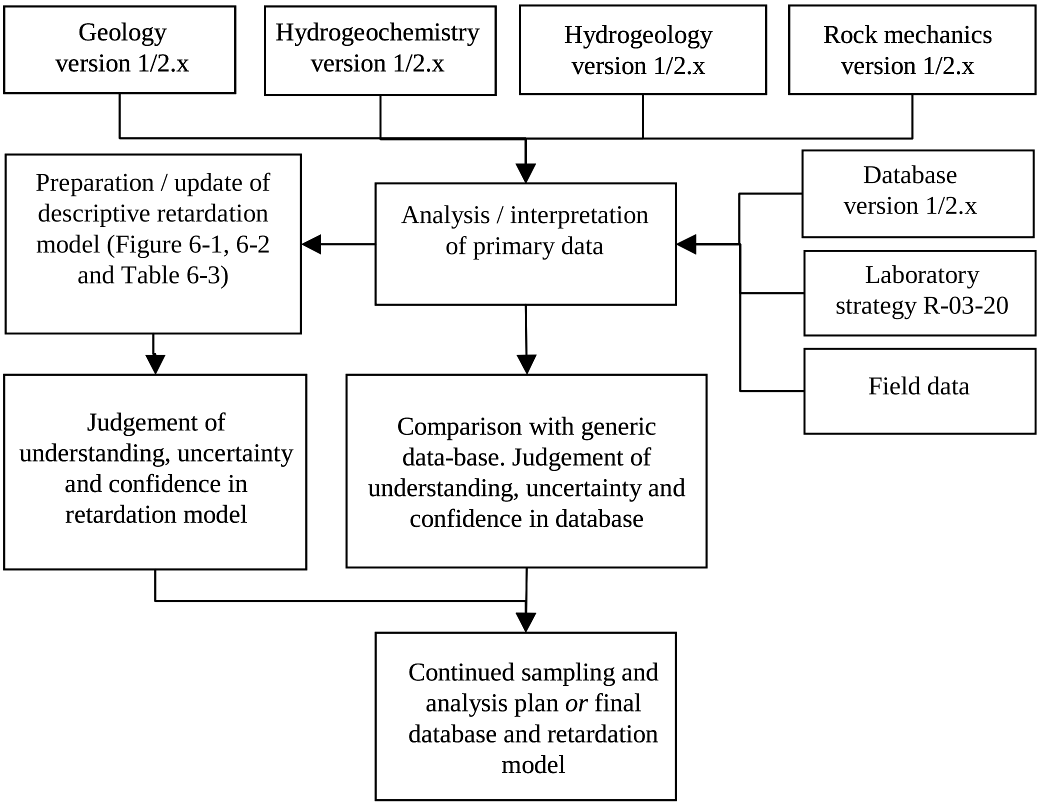


Figure 6-1. *Flow chart for the interpretation of primary data and preparation of the retardation model (from /Widestrand et al, 2003/; figure numbers refer to their report).*

The retardation model should be assessed with respect to the understanding and confidence in the underlying models, the database, and the retardation model itself, before it can be accepted. In particular, a description of the uncertainties should be provided.

6.3 Contents of the retardation model

The retardation model for a site consists of a number of data tables for the different units that are described. For a given site, the model may contain x number of tables for rock types, y tables for fractures and z tables for local minor fracture zones, which means that $x + y + z$ tables are delivered as input to the three-dimensional modelling. A schematic description of a retardation model is given in Figure 6-2. The parametrisation of a hypothetical fracture is illustrated in Figure 6-3, and an example of a data table is presented in Table 6-1.

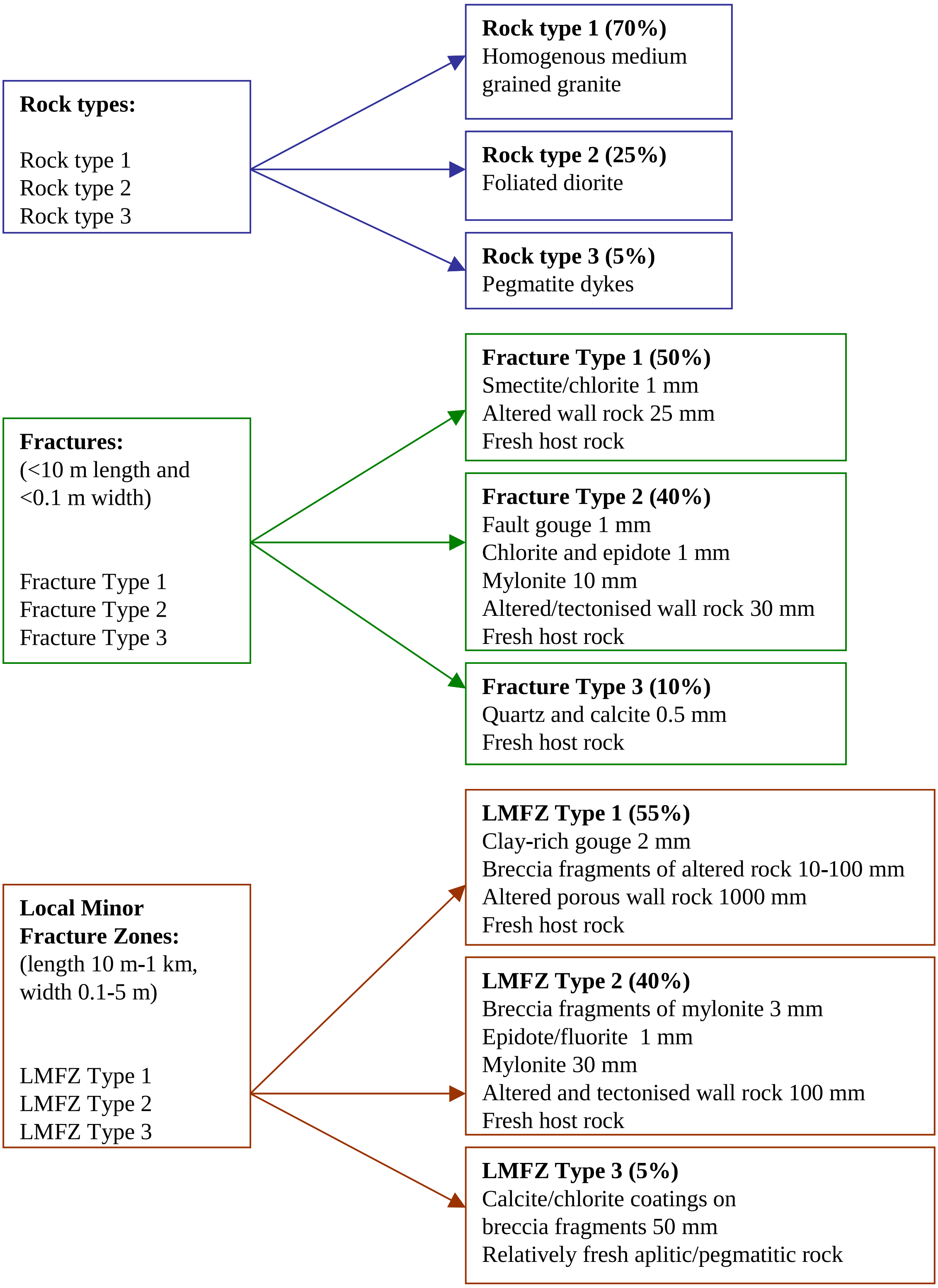


Figure 6-2. *Schematic description of the retardation model for a hypothetical site /from Widestrand et al, 2003/. The %-values is an estimation of the proportions of the rock, fracture or local minor fracture zone types within the site.*

Table 6-1. Hypothetical example of a compilation of retardation properties for a fracture in the retardation model /from Widestrand et al, 2003/.

	Gouge	Fracture coating	Mylonite	Altered wall rock	Fresh host rock
Distance[1]	1 mm	0–1 mm	1–10 mm	10–30 mm	30 mm –
Porosity[2]	0.5 (estimated open fracture voids)	0.10 (estimated) No gradient	0.03±0.01 (mean±1s) Linear gradient from 0.05 to 0.01 Cross-sectional log-normal distribution $10^{(-2.4\pm0.5)}$	0.008±0.002 (mean±1 st.dev.) Linear gradient from 0.01 to 0.005 Cross-sectional log-normal distribution $10^{(-1.7\pm0.5)}$	Data available in the data description for the host rock
Diffusivity[3]	5E–10 m^2/s (calculated)	2E–10 m^2/s (calculated)	1±0.3E–12 m^2/s (mean±1s) Linear gradient from 3E–12 to 7E–13 m^2/s.	5±2E–13 m^2/s (mean±1s) Linear gradient from 7E–13 to 3E–13 m^2/s.	Data available in the data description for the fresh host rock
Mineral content and grain sizes[4]	-	-	-	-	-
Sorption capacity[5]	-	K_d(Cs) for water type A: 5±2E–2 m^3/kg etc	K_d(Cs) for water type A: 1±0.5E–2 m^3/kg etc	K_d(Cs) for water type A: 8±3E–3 m^3/kg etc	Data available in the data description for the fresh host rock
Portion of conducting structure[6]	40%				
Transmissivity interval[7]	1E–6<T<1E–7 m^2/s				

1. Average/typical distance of e.g. the altered zone perpendicular to the fracture surface

2. Porosity can be given as estimated value, mean value with standard deviation or maximum variation width and as porosity distribution and porosity gradient.

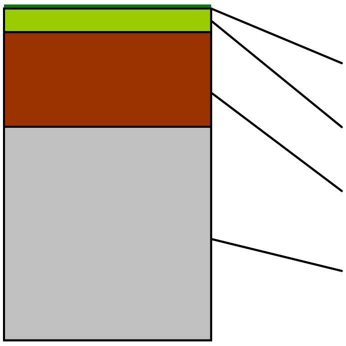
3. Diffusivity is given for HTO and calculated for sorbing species according to /Ohlsson and Neretnieks, 1997/. Surface diffusivity for sorbing species is also considered according to Ohlsson and Neretnieks.

4. Mineral contents should also include description of grain size distribution if possible.

5. The default value for species not listed in the table is the value given in the generic database. Data can be given for a certain species if this specie is interpreted to deviate significantly from the generic database. Correction factors may also be given for groups of elements according to the discussion in section 6.2.1 and 7.3.3 of /Widestrand et al, 2003/.

6. Describes for how large portion of the entire fracture size class at the site the given description is valid.

7. Typical fracture transmissivity interval based on data from flow logging of the sampled fracture intersections. This value and the fracture frequency can be used in transport modelling to link retardation properties to fracture transmissivity.



Thickness	Mineral/rock	Mean Porosity (-)	K_d(Cs) (m^3/kg)	D_e(Cs) (m^2/s)
0-1 mm	chlorite	0.05	5E-2	5E-12
1-10 mm	mylonite	0.02	1E-2	1E-12
10-30 mm	altered rock	0.01	8E-3	5E-13
30 mm -	fresh host rock	0.005	5E-3	2E-13

Figure 6-3. *Hypothetical example of fracture layer description and some selected parameters /from Widestrand et al, 2003/.*

6.4 Evaluation of data from in situ methods

Field data on retardation parameters should be included in the development of the retardation database and the retardation model. The in situ methods that produce mainly advection parameters, that is, multi-well tracer tests with non-sorbing (and weakly sorbing) tracers and groundwater flow measurements, are handled separately. This is because these measurements serve other purposes, such as to test the confidence in the hydrogeological description and to provide advection parameters for specific transport modelling tasks.

Concerning the multi-well tracer tests, it is recommended that a basic evaluation is performed, using the same model as in the TRUE Block Scale project (the "SKB-GESIGMA" model in Table 4-4; see also /Andersson et al, 2002d/). Additional modelling with other, more "advanced" tools is performed only if this evaluation shows large deviations between model results and measurements. Of course, other models will be used also if it is obvious that the experimental conditions deviate from the basic assumptions of the model, or if the particular test is directed towards processes or features that are not within the capabilities of the basic model.

6.5 Data evaluation during the Initial Site Investigation

During the Initial Site Investigation, very little site-specific retardation data will become available. This implies that the data will be insufficient for development of site-specific databases and retardation models in accordance with the strategy outlined above. Therefore, the site descriptive modelling of transport properties during the ISI phase will be based mainly on generic databases.

If the generic databases contain data of sufficient amount and quality, they could be used as a basis for development of preliminary retardation models through similar discipline-integrated evaluations as proposed for the primary site data. These models could be viewed as initial hypotheses as to the units that need to be described and their retardation properties, which are tested and updated when site-specific data become available. However, the level of complexity in the data evaluations during the ISI phase depends on the generic data, and will be decided based on an assessment of the database for each site.

Finally, it should be noted that in practise the distinction between data evaluation and three-dimensional modelling may not be as clear and definite as indicated in this report. In particular, the parametrisation of the rock units with retardation parameters will follow more or less directly from the retardation model, which implies that very little additional modelling work is required to “transform” the retardation model to a three-dimensional model of the rock units at the site. This is because the subdivision of the site into rock units is the main basis for the identification of typical, site-specific rock types. For the structures, however, modelling is required to associate the “type structures” (and combinations of them) in the retardation model with specific fractures and fracture zones at the site.

7 Three-dimensional modelling

7.1 Objectives

The three-dimensional transport properties modelling that produces parameters for radionuclide transport calculations consists of three main, inter-related activities; these modelling activities and their objectives can be summarised as follows:

A Descriptive modelling of retardation (diffusion and sorption) parameters of geological units (rock units and structures):

- to present parameters for further analyses of, primarily, spatial variability within the site descriptive modelling (input to analyses of flow paths),
- to present parameters for use in calculations performed by Safety Assessment (final product).

B Calculations of flow-related transport parameters for flow paths:

- to present parameters that illustrate the present-day conditions for advection and retention at the sites,
- to provide a basis for identifying rock volumes of unfavourable conditions for radionuclide transport,
- to quantify spatial variability in retardation parameters along flow paths
- to investigate uncertainties related to advection and the geometric description of fractures and fracture zones.

C Assessment of confidence and understanding:

- to describe the site-specific geoscientific understanding of factors that affect radionuclide retention,
- to present geological and hydrogeochemical evidence that supports the processes considered in the site descriptive model and alternative/complementary descriptions of radionuclide retention.

The preceding chapters describe the conceptual basis and the modelling tools (Chapter 4), the input data (Section 2.6, Chapters 3–5), and the data evaluations (Chapter 6), that constitute the basis for the three-dimensional modelling. In particular, some major methodological inputs are presented in Section 4.8. The aim of this chapter is to provide an overview of the planned modelling work, focusing on aims, procedures and guidelines, and not so much on detailed descriptions on how the various modelling tasks should be performed. Sections 7.3 – 7.8 are focused on Activities A and B above (quantitative modelling and parametrisation), whereas Activity C is discussed in Section 7.9 and also in Section 8.3.

7.2 Performing the work

The following general guidelines are proposed for the site descriptive modelling work:

- The evaluation of retardation parameters and the parametrisation of geological units with these parameters shall be performed by a group of experts who, in view of all the available information (including the generic data), develop retardation models and assign parameter values to structures and rock mass. This group should include geological and hydrogeological competence, as well as experts on retention processes and laboratory investigations of these processes. A close co-operation with experts on groundwater flow, flow-related transport parameters, and Safety Assessment is also required.
- The assessment of site understanding and model confidence related to retention will to large extent be based on data and other information collected and analysed in the process of retardation model development and parametrisation of geological units. Thus, essentially the same groups of experts will produce both the parametrisations and the supporting descriptions. However, it should be emphasised that the latter, more qualitative part is an important component of the overall modelling results.
- Flow-related parameters will be produced by particle-tracking simulations in groundwater flow models. The simulations are to be specified in Task Descriptions (TD). A TD lists SKB's general and specific objectives for the simulations, and specifies a minimum level of quality assurance in the model setup and expected output. The procedure for developing TD:s and the associated Activity Plans is described by /Rhén et al, 2003/, who also present a tentative TD example.
- Other quantitative transport modelling to be performed in support of the site descriptive modelling, cf. below, is organised within the site descriptive modelling projects. The modelling work is performed within the project groups or by external modelling teams.

With regard to the performance of the modelling work, the main messages to be conveyed here are the following:

- Expert groups should be formed for the data evaluations and the three-dimensional modelling of retardation parameters, including the support descriptions outlined above. These groups should contain all the necessary competences (cf. above). A close co-operation with the site characterisation organisations must also be secured.
- Groundwater flow modelling resources, that is, personal and computational resources, must be reserved for the calculations of flow-related transport parameters. Procedures for communicating specifications of modelling tasks (contents of TD:s) and simulation results between the groundwater flow modellers and site descriptive modelling teams must be established.
- The calculations of flow-related transport parameters require extended capabilities of the groundwater flow models, as compared to the present model versions. These extended capabilities include:
    - Integrations with spatially variable retardation parameters. This involves routines for handling these parameters (input and output routines), and for calculating additional flow-related parameters in the particle-tracking simulations.

  - Calculations of flow-related parameters for different geological units along the flow paths. For example, this may imply that the flow models must keep track of where (in what unit) the particle is at every time step of a simulation.

7.3 Stages of model development

The site descriptive models that will be produced during the Site Investigations are presented in Table 1-1. The three-dimensional modelling is here described as three different activities or stages:

- Modelling during the Initial Site Investigation (ISI).
- The first modelling stage of the Complete Site Investigation (CSI-Intact rock).
- The second modelling stage of the Complete Site Investigation (CSI-Structures).

The subdivision of the CSI modelling into two stages reflects both an increasing access to site data as the investigations proceed and a prioritisation with regard to the users. Specifically, it is assumed that a “complete” retardation model and a detailed parametrisation of structures in line with the Task 6C approach outlined in Section 4.8 will be performed during the second CSI stage. During the first CSI stage, simplified parametrisations are developed.

From a user perspective, the first, “CSI-Intact rock” stage is focused on the parameters required for Safety Assessment. The second, “CSI-Structures” stage of more detailed modelling of the structures emphasises the geoscientific understanding of the site, especially spatial variability and the role of altered materials near structures. However, the results of the detailed modelling in the “CSI-Structures” stage may have implications also for Safety Assessment. It should be noted that the two stages are not associated with particular model versions; they address different user needs, and may be developed for each model version 2.x if data becomes available.

The two CSI stages are focused on:

1. Parametrisation of intact rock (long-term/SA time perspective), and a basic subdivision of retention along flow paths into contributions from stochastic and deterministic structures (that is, “small” and “large” structures).
2. Detailed parametrisation of the (individual) structures along the lines of Task 6C and quantification of the resulting longitudinal variability along flow paths, and assessment of transverse variability due to “stratification” of altered rock and the associated time dependence of the retardation capacity.

7.4 Main modelling components and tools

The inputs and modelling components from Primary Data evaluations and contributions from other disciplines can be summarised as follows:

- **The retardation model** that constitutes the final product of the Primary Data evaluation: diffusion and sorption parameters for rock units, and a description of "type structures" in terms of layer thickness and retardation parameter values for the layers.

- **The geological description of the site:** a geometrical description of rock units and deterministic structures, geological parameters, including mineralogy, and a DFN description of the stochastic fractures.
- **The hydrogeochemical description of the site:** a description of the typical water compositions at site, including their spatial distribution, identified water/rock interactions, and studies of fracture mineralogy and trace elements in the matrix near fractures.
- **The hydrogeological description of the site:** a description of deterministic structures, HCD (geometry and hydraulic parameters), and stochastic fractures within HRD (DFN parameters of conductive features).
- **Groundwater flow models**: local and regional scale flow models developed with DarcyTools and CONNECTFLOW.
- **Mathematical transport models:** "simple" routines for averaging flow-related parameters along trajectories, streamtube and trajectory models (e.g. FARF31, LaSAR), and, possibly at later stages, coupled models for process modelling.

The roles and interactions of these modelling components in the different stages of the site descriptive modelling are further described below.

7.5 Methods and modelling guidelines

7.5.1 Parametrisation of geological units

The retardation model will become more "mature", detailed and site-specific as the Site Investigations proceed. In view of this development, two main "complexity levels" of the parametrisation of the structures can be identified:

- *Deterministic assignment of retardation parameters to the structures.* For example, a single "type structure" could be assigned to all stochastic structures within a rock unit, whereas the deterministic structures are handled on a case-by case basis. In a more detailed deterministic parametrisation, different type structures can be assigned to different stochastic structures based on, e.g. a size cut-off.
- *Stochastic assignment of type structures and combinations of type structures:* Type structures and the associated retardation parameters are assigned to individual stochastic structures based on correlations with other fracture properties, e.g. the size, as outlined above. Deterministic structures can be "constructed" as combinations of basic type structures. Thus, the parametrisation can describe spatial variability within the larger structures, through, e.g. a "complexity" parameter (Section 4.8), whereas the smallest structures consist of a single type structure and hence are associated with a single set of retardation parameters.

It should be noted that the terms "deterministic" and "stochastic" refer to the assignment of properties, not to the resulting descriptions. This means that a stochastic description of spatial variability at the "sub-structure scale" is possible in either case, depending on the data provided in the retardation model. Similarly, the intact rock within the rock units can be parametrised by deterministic values or stochastic distributions. Furthermore, the stochastic description may include spatially uncorrelated or correlated parameters.

Modelling guidelines

The main modelling guidelines can be summarised as follows:

- The three-dimensional modelling of retardation parameters focuses on the present situation, that is, on parameter values that correspond to the present geological, hydrogeological and hydrogeochemical conditions.
- The subdivision of the model domain into different rock units provides the basic geometric framework for assigning parameter values to the intact rock and the stochastic structures. In some cases, the interpretations of transport properties may suggest different subdivisions of the model domain. It is foreseen that these modifications primarily will result in simplified model domains.
- The parametrisation of the intact rock (the unaltered rock mass) will describe spatial retardation variability on three basic scales: (i) variability/differences in (sets of) parameter values for different rock units, (ii) spatial variability within individual rock units, and (iii) spatial variability within individual rock types. For the description of retardation parameters within individual units, the aim is to develop a description in terms of statistical distributions. This implies that spatial variability of individual parameters, as well as correlations between different parameters, should be investigated and described. However, it should be noted that the required degree of detail is determined by the users (by the acceptable uncertainty in the parametrisation).
- The Task 6C methodology is proposed as the general framework for the parametrisation of structures with retardation parameters, although simplified approaches will be taken at early stages. It should be emphasised that the complexity of the modelling work depends strongly on the (interpreted) site-specific conditions, and that the methodology will be further developed based on experiences gained from the ongoing work within the Äspö Task Force and the Site Investigations.
- The parametrisation of the stochastic structures should follow the rock units, or a simplified subdivision of the model domain if appropriate. This means that different type structures or combinations of type structures could be assigned to fractures in different rock units. Retardation parameters are assigned to the individual structures within each unit by either deterministic or stochastic procedures.
- The deterministic structures are handled on a case-by-case basis in a deterministic assignment of retardation parameters, or are parametrised in a stochastic procedure based on the complexity of the structures. Spatial variability within the structures can be considered in either case.
- The uncertainties associated with the retardation parameters should be described. These uncertainties include data uncertainties associated with measurements and interpretations, as well as conceptual uncertainties related to the underlying process description, see Section 7.9.

7.5.2 Methods and guidelines for obtaining flow-related parameters

Different transport modelling approaches and methods for quantifying flow-related parameters are discussed in Chapter 4 and Appendix A. The flow-related parameters, which are integrated parameters describing advection and retardation along flow paths in the fractured rock, are obtained from simulations with groundwater flow models. Different methods can be used when calculating transport parameters in connection with flow simulations. During the site descriptive modelling, the following main alternative/complementary methods or "complexity levels" will be considered:

- Calculations of hydrodynamic parameters (t_w and F) in the groundwater flow models and separate modelling of the parameters that describe the effects of diffusion and sorption. This implies that only hydrodynamic information is "extracted" from the flow models. Note that this hydrodynamic information may concern entire flow paths (usually the case) or parts of flow paths that coincide with different units or domains in the rock.
- Calculations of integrated hydrodynamic and retardation parameters in the groundwater flow models. To enable integrations of retardation parameters along the flow paths, diffusion and sorption parameters must be transferred to the flow models.
- Coupled flow and transport modelling, which means that "actual process modelling" is performed, rather than integrations of parameter values along flow paths.

In the site descriptive modelling, flow-related parameters will primarily be calculated by particle tracking and integrations along particle trajectories. The preferred modelling method for the combined advection and retardation parameters, at least in the early stages of modelling, is to "extract" hydrodynamic information (on entire flow paths as well as parts of flow paths), and then perform "mathematical transport modelling" separately. In, for example, a case where different retardation parameters apply to different rock units, the flow modellers should deliver t_w- and F-values for each rock unit along each path.

Flexibility is the main reason for this preference; if relevant data on t_w and F are available, also for different geological units within the model domain, the effects of different retardation parameter combinations can easily be investigated. The main alternative approach, in which transport parameters are transferred to and integrated within the flow models, requires a new parametrisation and flow simulation for each set of retardation parameters. The obvious disadvantage of the "extraction" method is that much more output data is obtained from the flow models than if all analyses are performed internally. Clearly, it cannot be applied in the same way when a complete parametrisation of all individual structures has been performed. However, a similar approach can be taken, where hydrodynamic parameters are integrated for the different type structures along the paths.

Modelling guidelines

The main modelling guidelines can be summarised as follows:

- Flow-related parameters will be calculated for the present flow and retardation conditions. Although transient conditions are considered in the groundwater flow modelling, transport calculations are performed for steady flow (in "snap shots" of the flow field). Other scenarios, involving, e.g. future hydrogeochemical conditions (and hence, possibly, different diffusion and sorption parameters), or transport in transient flow, will be handled by Safety Assessment.

- The modelling tasks should be specified in Task Descriptions (TD) to the groundwater flow modellers, see Section 7.2. The TD:s should include the required transport-related specifications, primarily a description of boundary conditions (injection locations for particles) and output parameters (performance measures).
- Particle tracking in DFN-based models is the main method for calculating flow-related parameters. Other methods will be used for comparative purposes. Specific guidelines on the calculations of the *F*-parameter are given below.
- In cases where spatially variable retardation parameters are considered, the combined advection and retardation parameter groups can be calculated either directly in the flow models, which implies that these models must be parametrised with retardation parameters, or in a separate modelling step that uses hydrodynamic parameters extracted from the particle tracking simulations. Also in the second case, the flow models must contain information related to retardation, in order to enable calculations of integrated parameters for different units or type structures. For example, "identifiers" for the different units could be used to control the integrations. Whereas the "direct method" is conceptually straightforward, the "extraction method" offers advantages when considering, e.g. additional sets of retardation parameters. It is proposed that the "extraction method" method is further developed during the Site Investigations.
- For the retardation parameters, two basic alternatives are considered: (i) a parametrisation based on the diffusion and sorption properties of the intact rock, and (ii) a parametrisation based on the properties assigned to structures (type structures consisting of several layers). In the first case, the variability along the flow paths is given by the parameters assigned to the rock units, whereas in the second case it is determined by the parameters of the structures. For calculations with the second type of parameters, which include different parameters for different layers in the matrix, a selection or modelling that provides representative (or otherwise relevant) parameter values is required. In other words, a "pre-processing step" is needed to identify the retardation parameters to be used in the modelling.
- Spatial variability along flow paths/particle trajectories will be described statistically. Two different "modes" of randomness can be considered: (i) spatial variability in flow and transport parameters, resulting from the stochastic parameters assigned to the conductive structures in the DFN model, and (ii) "branching" at fracture intersections, which reflects different probabilities of different down-gradient paths in the stochastic fracture network. Since different types of randomness affect the calculation results, the specification of adequate output statistics (e.g. "pooled" statistics, single-realisation statistics, or statistics for a single injection location) is important. This specification is given in the TD for the simulations.
- Spatial variability in the transverse direction (into the rock matrix) could be viewed as corresponding to time-dependent ”effective” retardation parameters in a model that does not explicitly account for transverse variability. It is proposed that the retardation parameters that are used in calculations addressing the time dependence of retardation are obtained through selection or separate modelling of "effective"

parameters. In the latter case, either the analytical TRUE Block Scale approach /Cvetkovic and Cheng, 2002/ or the fully numerical version of FARF31 can be used.

- The FARF31 model is based on an advection-dispersion approach, and the model requires input of the dimensionless Peclet number (*Pe*) that quantifies dispersion (Table 4-1). Dispersion is a scale-dependent concept (see discussion in Section 4.3.2), and hence the *Pe*-value should depend on the transport problem at hand. When modelling transport from single canister positions, dispersion should be "small" ("large" *Pe*), whereas dispersion in other transport scenarios should be handled in accordance with the guidelines proposed by /Andersson et al, 1998a/.
- Uncertainties in the flow-related parameters should be described. The main uncertainties are related to the transport parameters and the underlying geological, hydrogeological and hydrogeochemical models. Specific guidelines for managing uncertainties are provided in Section 7.9.

Guidelines for calculating the *F*-parameter

The transport resistance, here referred to as the *F*-parameter, has been identified as an important parameter for Safety Assessment /Andersson et al, 2000; SKB, 2001b/. Different methods for quantification of *F* have been employed in the past. A major distinction can be made between DFN-based methods, in which the required geometric information is obtained directly from the fracture network, and methods that use travel times from flow models and independent quantifications of geometric parameters (usually a "flow wetted surface" obtained from fracture statistics). However, there is no general consensus on how to quantify the *F* parameter. In the site descriptive modelling, *F* will be calculated in DFN simulations. The following guidelines should be considered in this work:

- Different DFN-based methodologies will be employed: (i) direct simulations in the fracture networks, where geometric information (apertures, widths and lengths of pipes, channels or fracture planes) is recorded along the particles trajectories; (ii) mixed DFN/SC approaches. In DarcyTools, which is of the second category, local *F*-values are calculated for each element in the SC description, and integrated *F*-values are obtained by integrating the local values along particle trajectories.
- In DFN calculations, additional geometric assumptions are often made. These assumptions concern the relation between the total (geometric) surface areas or apertures and the corresponding "effective" values for transport, which quantify the fractions that take part in the transport processes. Different assumptions can and should be made in different models. No specific recommendations are proposed here as to what might be "correct" assumptions. However, all assumptions on "efficiency parameters" must be clearly stated, in order to facilitate comparisons between different models. In this context, it may also be noted that absolute values of *F* are more important for SA, where comparisons between different sites will be made, than for the site descriptive modelling, which primarily seeks to illustrate differences within sites.

The highest level of complexity in the DFN-based calculations is attained when considering spatial variability within the individual fracture planes. Such simulations could provide a basis for calculating, rather than assuming, the effective widths (or equivalent geometric parameters) of flow paths. It is suggested that this type of detailed simulations are performed as separate research activities. Based on the results of these activities, it can be decided whether to perform detailed simulations also within the framework of the site descriptive transport modelling.

7.6 Transport properties modelling during ISI

The data and models that will become available during the Initial Site Investigation (ISI) stage, and thus constitute the baseline for the modelling at that stage, can be summarised as follows:

- Only very limited site-specific retention data will be available, which means that the modelling must be based on generic/historic data.
- Local scale groundwater flow models will be developed, which means that hydrodynamic flow-related parameters can be calculated.

The objectives of the three-dimensional modelling are to:

- identify unfavourable transport conditions and units/structures that should be prioritised for further investigations;
- provide a preliminary description ("initial hypothesis") as to the diffusion and sorption properties;
- provide hydrodynamic transport parameters (F and t_w) for illustration of present-day site conditions for advection and retention.

The achievable degree of detail in the preliminary description of the retardation properties depends on the quantity and quality of the generic data. In particular, parameter values are required for materials interpreted to be "sufficiently similar" to those found within the geological units at the site. The available generic data will be compiled and assessed. Based on this assessment, it is decided if a sufficient basis exists for the development of a "preliminary retardation model" along the lines of /Widestrand et al, 2003/, or if a simplified description should be devised.

Thus, the modelling tasks are to develop a "preliminary retardation model" and assign parameter values to the geological units based on this model and the geological description, or to develop a simplified description/overview of the retardation properties. In addition, particle-tracking simulations, focused on the hydrodynamic parameters, should be carried out. In view of the objective to identify unfavourable conditions, it is proposed that these simulations should use release locations (stating positions of particles) that are evenly distributed within the entire local model area at repository depth, or within selected sub-areas. It follows that the required capabilities of the groundwater flow models are that they should be able to integrate and report travel times and F-values for entire flow paths.

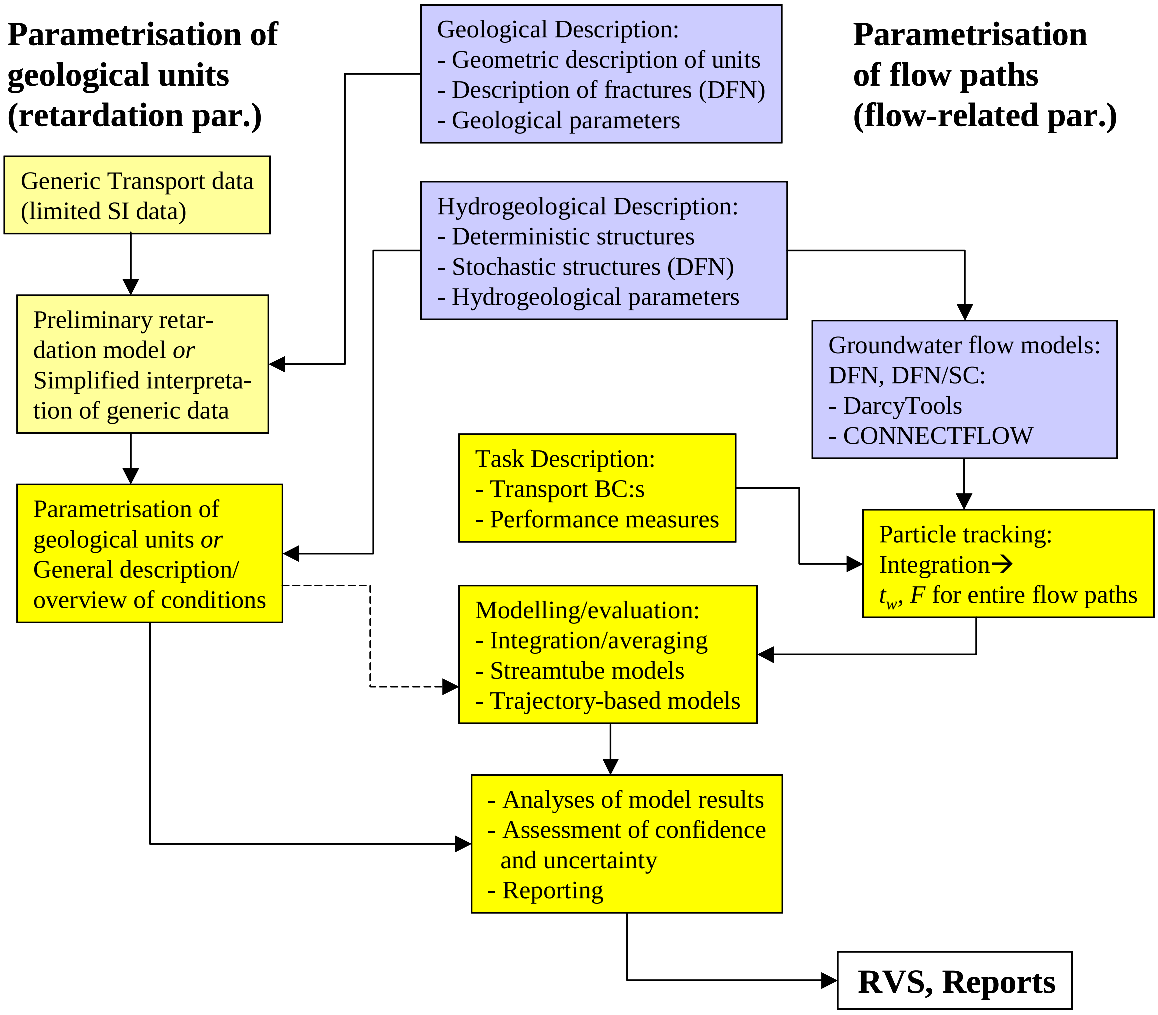


Figure 7-1. *Working methodology for three-dimensional modelling during the Initial Site Investigation. Yellow boxes indicate activities within the three-dimensional transport properties modelling, light yellow/beige boxes other transport inputs and activities, and blue boxes models produced within other disciplines.*

The three-dimensional modelling during the ISI stage is illustrated in Figure 7-1 above, using the modelling components described in Section 7.4. It can be seen that the parametrisation of geological units with retardation parameters and the parametrisation of flow paths with flow-related parameters are handled as more or less separate activities. As indicated by the dashed connector, retardation parameters may be used in "lumped" calculations of combined advection and retardation parameters for the flow paths. The alternative approaches to the description of the retardation properties are also indicated in the figure. Clearly, it would be an advantage if a preliminary retardation model and parametrisation of the units could be produced in the ISI modelling, as to provide a basis for sampling and testing at later stages.

7.7 Transport properties modelling during CSI – Intact rock

Site-specific retardation data will become available during the Complete Site Investigation (CSI). However, the amount of data will increase successively as the investigations proceed. This implies that the uncertainties associated with the modelling will decrease from one model version or stage to the next, provided that effective investigations are performed, such that different "complexity levels" in the modelling are appropriate at different stages.

As described in Section 7.3, we consider two basic CSI stages of descriptive modelling. In the first stage, only a limited amount of site-specific transport data is assumed to be available. The data is insufficient for development of a "complete" retardation model and for parametrisation of the structures in accordance with the methodology outlined in Section 4.8.1 at a reasonable level of uncertainty. Thus, the modelling is focused on the intact rock mass, which is consistent with a SA time perspective (or at least with common assumptions in SA modelling). In addition, a basic analysis of the retention capacity along different types of structures, that is, stochastic and deterministic structures, is proposed.

The objectives of the three-dimensional modelling in the "CSI-Intact rock" stage are to:

- describe the longitudinal (along flow paths) variability in the retardation properties of the intact rock, thereby providing retardation parameters for SA;
- perform a first analysis of the retardation capacity of different types of structures, focusing on a quantification of the relative contributions of stochastic and deterministic structures to the total retardation capacity;
- provide updated/refined hydrodynamic parameters (F and t_w) for illustration of site conditions.

As compared to the trajectory simulations during the Initial Site Investigation, the updated simulations could reflect developments in the hydrogeological description and the flow models and/or the geological and hydrogeochemical models, and a refined description of the transport boundary conditions (e.g. focusing on areas of specific interest).

The modelling tasks include:

- A simplified, deterministic parametrisation of stochastic and deterministic structures.
- Statistical analyses of retardation parameters and parametrisation of the intact rock within each rock unit. An important aspect of this work is to determine whether and to what extent (resolution) spatial variability needs to be considered.
- Trajectory simulations for "extraction" of hydrodynamic parameters (Section 7.5.2): (i) calculations of t_w and F for different rock units along the flow paths; (ii) calculations of t_w and F in the stochastic fractures (i.e., t_w- and F-values when the particles reach the larger, deterministic structures).
- Transport modelling (calculations of transport parameters by separate integration and averaging of characteristic parameter groups): (i) calculations of integrated characteristic parameters for the intact rock and averaging of retardation parameter groups; (ii) calculations of integrated characteristic parameters for stochastic and deterministic structures.

It follows that a sufficient amount of retardation data for intact rock must be available for performing these modelling tasks. However, data and general information on spatial variability in these parameters can to some extent be imported from other sites. Furthermore, interpreted "typical" fractures and their retardation parameters (within each geological unit), and first estimates of retardation parameters for the deterministic structures are needed. For the particle-tracking simulations, the groundwater flow models should have capabilities allowing calculations of hydrodynamic parameters for different geological units along the flow paths.

The three-dimensional modelling during the first CSI stage is illustrated in Figure 7-2. It can be seen that the retardation parameters and the hydrodynamic parameters are "imported" to a separate transport modelling step. As discussed in section 7.5.2, an alternative would be to parametrise the flow models with retardation parameters and integrate the combined advection and retardation parameters there. Furthermore, it is indicated in the figure that alternative methods will be used to calculate flow-related parameters (primarily *F*). The alternative methods that could be used include the "simple" estimators mentioned in Section 4.8.2, as well as calculations based on Channel Network and classical SC modelling.

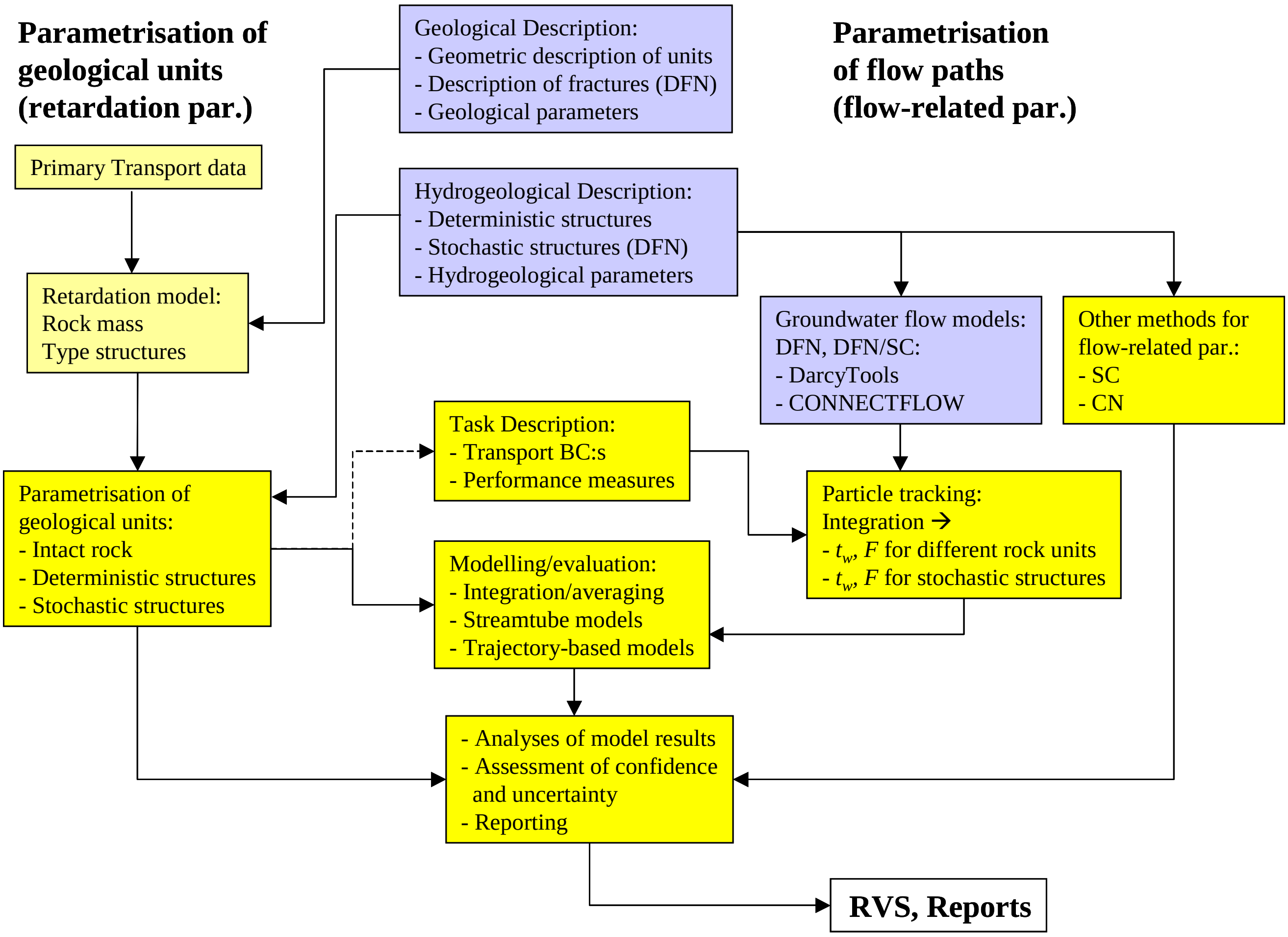


Figure 7-2. *Working methodology for three-dimensional modelling in the "Intact rock" modelling stage of the Complete Site Investigation. Yellow boxes indicate activities within the three-dimensional transport properties modelling, light yellow/beige boxes other transport inputs and activities, and blue boxes models produced within other disciplines.*

7.8 Transport properties modelling during CSI – Structures

In the second CSI stage, the aim is to develop a “complete” parametrisation of the structures, in accordance with the methodology outlined in Section 4.8.1. The parametrised models will be used to address the geoscientific understanding of the site, to study the effects of spatial variability in retardation parameters, and to produce transport parameters for SA. An important aspect of this work is to analyse the temporal evolution of the “effective” diffusion and sorption parameter groups associated with transverse spatial variability. Based on such analyses, it can be determined whether the retardation parameters of the intact rock provide a realistic description in the SA time perspective. Furthermore, the intact rock-based parametrisation of rock units and flow paths will be updated.

The objectives of the three-dimensional modelling in the “CSI-Structures” stage are to:

- develop detailed parametrisations of the stochastic and deterministic structures that describe the longitudinal and transverse spatial variability in sorption and diffusion parameters in stochastic realisations of the groundwater flow models;
- perform detailed analyses of the effects of spatial variability and temporal evolution in characteristic advection and retardation parameters;
- provide updated/refined hydrodynamic and retardation parameters for site understanding.

Thus, the modelling tasks include:

- A “complete” parametrisation of structures using site-specific “type structures” and a stochastic methodology based on correlations with DFN properties (e.g. structure size). In this procedure, retardation parameters are assigned to each member of the fracture population in each considered realisation of the DFN model. This implies that an additional stochastic parametrisation step is required. These detailed, possibly multi-realisation models are used as a basis for calculating flow-related parameters, and in further transport analyses. A complete description including all (individual) fractures and their parameter values cannot be included in the site descriptive RVS model. However, the site descriptive model should include all the data required to perform the parametrisation.
- Transport modelling, including trajectory simulations, integrations of retardation parameters along flow paths, and modelling of transverse spatial variability. As described in Section 7.5.2, transverse variability will be handled separately, thereby providing input to the trajectory simulations/integrations in the form of a selection of specific layers or effective parameter values for the different “type structures”. Transport modelling can be performed in separate transport models, using “extracted” trajectory information, by “direct” integrations of both advection and retardation in the flow, or in fully coupled flow and transport models. Whereas trajectory simulations of hydrodynamic parameters and separate transport modelling is considered the main modelling approach, it is suggested that a multi-model approach is taken to quantify uncertainties and improve the understanding of the sites (cf. below).

The main interactions between model components in the three-dimensional modelling during the second CSI stage are illustrated in Figure 7-3. The retardation data required for the site descriptive modelling at this stage includes a “complete” retardation model and statistical information about the intact rock properties in the different rock units. The required capabilities of the groundwater flow models include functions for joint hydrogeological-retardation parametrisation, and for handling retardation parameters during the simulations. Different models and modelling approaches could, and should, be used in the CSI transport modelling. For example, parallel modelling by different modelling teams could contribute to the understanding of the site and provide a basis for evaluating model-related uncertainties.

Radionuclide transport will be investigated both for the purposes of site descriptive modelling and by Safety Assessment. Since both activities study various aspects of uncertainty and sensitivity, the distinction between them may not be completely clear (see Section 2.3). However, the site descriptive modelling is concerned primarily with the present conditions and modelling based on site-specific, measured data.

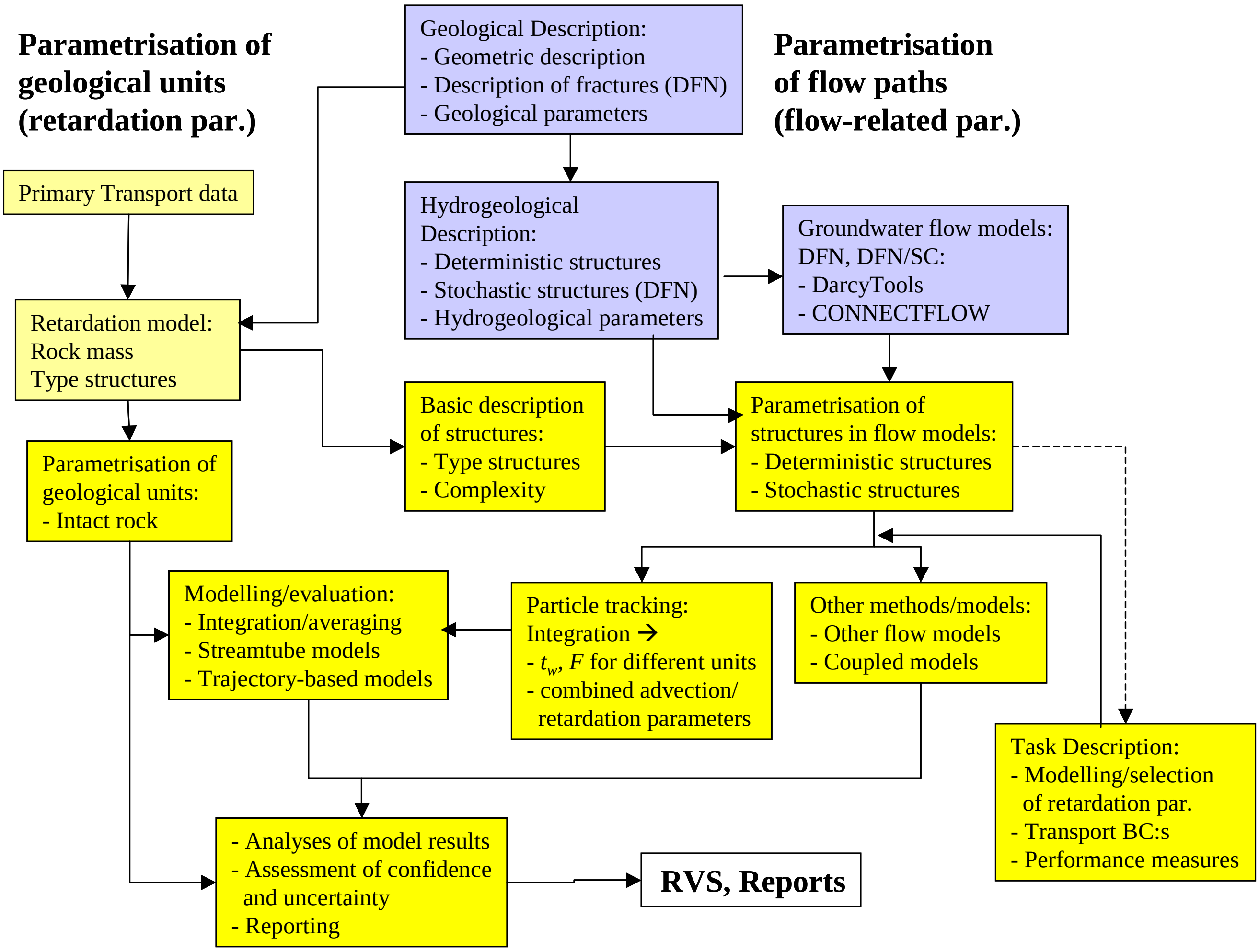


Figure 7-3. *Working methodology for three-dimensional modelling in the "Structures" stage of the Complete Site Investigation. Yellow boxes indicate activities within the three-dimensional transport properties modelling, light yellow/beige boxes other transport inputs and activities, and blue boxes models produced within other disciplines.*

Although the future development of the parameters in the descriptive model could be discussed in connection with the Site Description, quantitative analyses of future scenarios are to be performed by SA only. Furthermore, the flow paths investigated and reported within the site descriptive modelling, as determined by the release locations of particles, are selected to illustrate present site conditions and for developing the geoscientific understanding of the sites, whereas specific repository layouts are considered by SA only.

7.9 Assessment of uncertainty, confidence and understanding

7.9.1 Uncertainties in transport models

An overview of uncertainties associated with the transport properties modelling is given in Section 2.9. In the following, guidelines for the assessment and quantification of *conceptual uncertainties* and *data uncertainties* are given.

- Data uncertainties associated with laboratory measurements of retardation parameters should be quantified. These include uncertainties in the individual measurements (measurement and interpretation errors), uncertainties related to the application of the methods, and inconsistencies in measurements with different methods. Guidelines for handling these uncertainties are given by /Widestrand et al, 2003/.

- If in situ measurements of retardation parameters are performed (Section 5.1.2), the results should be evaluated together with the laboratory results, in order to develop the basis for a description of spatial variability and its associated uncertainty.

- The evaluation of Primary Data, in particular, the development of the retardation model, is based on interpretations of what constitutes “typical” rock mass units and structures, and “typical” geological materials within and in connection with these units and structures. These interpretations are to some extent based on expert judgment, and uncertainties are difficult to quantify. Internal and external reviews will be an important tool for uncertainty assessment of these interpretations. However, the methods for this type of assessment should be further developed, especially since the uncertainty in the retardation model is strongly related to the need for additional measurements.

- Spatial variability in parameter values is generally an important source to data uncertainty. For a particular parameter, the actual (unknown) parameter variations, the measurement, modelling and transport scales, and the importance of the parameter for the transport problem at hand, determine the need for detailed analysis of the parameter. Spatial variability in the primary transport parameters will be described when parameters are assigned to the geological units, but the related uncertainty is quantified primarily in the analysis of flow-related parameters and characteristic parameter groups. The flow-related parameters are also affected by spatial variability and uncertainty in the description of flow. In the evaluation of the trajectory simulations, a clear distinction must be made between uncertainty and physical spreading. The scale of the flow model is important for this analysis. The model scale determines the resolution of the particle tracking simulations, and hence the scale at which variability is described explicitly.

- Uncertainties in the geological and hydrogeological descriptions can be analysed by means of alternative models. Since the transport modelling uses the geological, hydrogeological and hydrogeochemical descriptions as input, the alternative models produced within these disciplines should (strictly) be propagated and result in alternative transport models. However, the development of alternative models is resource demanding, and, presumably, not always motivated. The alternative models presented by the other disciplines should be examined by the transport modelling teams, in order to assess the implications for the transport description. Based on this assessment, it will be decided whether an alternative transport description should be developed, and which features, parts or parameters of the model that need to be re-analysed.
- Conceptual uncertainties related to the primary transport processes and parameters originate from the basic assumptions of the main modelling approach described in Section 4.3.1, as well as from other model simplifications. Although difficult to quantify, these uncertainties should be described in the transport description. The use of parallel modelling/alternative approaches, as suggested in Section 7.8, could involve alternative retention models, thereby relaxing, e.g. the assumption of linear equilibrium sorption (see Section 4.4). Other model simplifications and potential inconsistencies that should be addressed, although probably not in a quantitative fashion within SI, are:
    - *The assumption of steady flow in the transport calculations.* Transient flow implies that different discharge points will be obtained for solute particles that are released at fixed locations at different times. Furthermore, solutes with different retardation properties could follow different paths through the rock, and also have different exit points at the rock surface. The quantitative analysis of the effects of transient flow is handled by SA. Important aspects of this analysis would be to investigate the sensitivity of the discharge pattern to the transients, especially whether the same larger structures (if such are present) continue to determine the discharge pattern, and if different radionuclides have significantly different exit points.
    - *The assumption of homogeneous fractures.* As mentioned in Section 7.5.2, detailed simulations where heterogeneity within individual fracture planes is considered could provide important information on the flow distribution and the conditions for mass transfer. It is suggested the usefulness of this type of simulations is evaluated in separate research activities.
    - *Modelling of chain decay under conditions of spatially variable retardation*. The radionuclides that are formed in chain decay reactions each have different “starting positions” along a flow path. These “starting positions” also differ from that of the nuclides that are not subject to such reactions. If retardation properties are spatially variable along the flow path, this implies that different solutes will “sample” different distributions of retardation parameters. In FARF31, chain decay is modelled with uniform retardation parameters. This apparent inconsistency could be investigated using the numerical version of FARF31.
    - *Modelling of colloid transport.* Enhanced radionuclide transport through sorption onto and transport with colloids has been proposed as an explanation of observed spreading of strongly sorbing radionuclides /Kersting et al, 1999/. A

comprehensive assessment of the potential for colloid-enhanced transport in connection with SKB’s concept for waste disposal was carried out by /Klos et al, 2002/. Furthermore, /Cvetkovic, 2003/ performed a theoretical study using input data from Äspö HRL. The general conclusion that can be drawn from these studies is that site-specific data are required to make a first assessment of the potential significance of colloids and the need for transport modelling involving colloids. Colloids are studied within the Hydrogeochemistry programme, but transport modelling is presently not included in the evaluations of this data. Specific investigations could be performed in co-operation with Hydrogeochemistry, if motivated by experimental evidence.

- The various existing methods for determining the transport resistance, *F*, involves aspects of both conceptual and data uncertainty. The main tool for quantification of conceptual uncertainty is to compare the results of trajectory simulations in different groundwater flow models (DFN, SC and DFN/SC), and to compare trajectory simulations with other modelling results and estimators. Data uncertainties associated with spatial variability are quantified by means of statistical analyses of *F* distributions calculated in multiple realisations of the flow field. Uncertainties related to alternative geological and hydrogeological models could also be important for the analysis of *F* values. These uncertainties can be assessed by comparing the *F* distributions obtained from the corresponding alternative groundwater flow models, provided that such models are developed.

7.9.2 Assessment of confidence in transport models

The confidence in a descriptive model is the total assembly of motives, indications and arguments in support of the model /Andersson, 2003/. The confidence is essentially a qualitative entity. It should be judged for the discipline-specific descriptions, as well as in a joint confidence assessment. The judgment of confidence involves analyses of data sources and interpretations, consistency between disciplines, and comparisons with previous model versions. Guidelines for these analyses are given by /Andersson, 2003/.

The ability to explain current site conditions and ongoing natural processes is important for the confidence in a descriptive model. For obvious reasons, however, direct evidence of transport properties and processes under conditions directly corresponding to the radionuclide release scenarios modelled by SA cannot be obtained. From this point of view, the transport description can be regarded as “a model of other models” that largely relies on the observations that support the underlying models (primarily those presented by Geology, Hydrogeology and Hydrogeochemistry). Therefore, different types of more or less indirect evidence for transport processes must be utilised, where, e.g. uncertainties related to sources and differences in terms of time scales are important for whether the indirect evidence is representative for hypothetical, future transport conditions.

Transport processes in the field can be observed under controlled, disturbed conditions in multi-well tracer tests. However, although tracer tests could be used to quantify both advection and retention parameters, we consider them mainly as a tool for investigating the confidence in the hydrogeological description and for specific studies of advection parameters (see Section 8.1). As discussed in Chapter 5, the site descriptive transport modelling will to some extent use diffusion and sorption data from previous investigations at the sites and elsewhere, especially in the early stages of model development. Therefore, judgment of the methods employed to obtain this generic data and the correspondence of site conditions are important factors for the confidence of the models.

Data, data evaluations and modelling work within other modelling disciplines provide the basis for assessing the confidence in the description of radionuclide retention. Specifically, the information collected and evaluated in order to describe model confidence should include:

- Evidence supporting the *actual occurrence of matrix diffusion and sorption* at the investigated sites, that is, observations showing that these processes are or have been active.
- Evidence supporting the *actual occurrence of other retention processes* (processes that increase or decrease the overall retention effect).
- Evidence supporting that matrix diffusion and sorption, and/or other retention processes, *could occur* at the investigated sites, that is, observations of site conditions that could be used, e.g. for developing analogies with other sites.
- Site data and models that could provide a basis for developing *alternative process-based retention models* (see Chapter 4).

The main data sources are Geology (mineralogy) and Hydrogeochemistry (water compositions in fractures and matrix, identified water/rock interactions). /Andersson et al, 2002c/ (see Chapter 7 in their report) provide an example of how retention can be described using diffusion and sorption data in conjunction with available geological and hydrogeochemical information.

In the site descriptive modelling, the joint geological-hydrogeochemical analyses of fracture minerals, fracture-filling materials, and trace elements that will be presented by Hydrogeochemistry will be important for the assessment of confidence and the description of process understanding. An important aspect of these investigations is the analysis of trace elements in the fracture minerals, which may provide site-specific evidence of matrix diffusion /cf. Landström et al, 2001/.

Previous studies of natural analogues present methodologies and results with relevance for confidence assessment, see /Bruno et al, 2001/. Furthermore, matrix diffusion is modelled by Hydrogeology in groundwater flow simulations of density-dependent flow. This implies that observations made in connection with these modelling efforts also could have implications for Transport, such that they give supporting evidence of matrix diffusion.

Quantitative, process-based analyses using alternative retention models are potentially useful for supporting and complementing the description produced by the main modelling approach considered here. In particular, process-based modelling of sorption could provide a complementary means for quantifying sorption parameters, thereby enabling comparisons to and a rational way of extrapolating the experimental data produced within the Site Investigation laboratory programme. However, our present view of the potential for using such models within the site descriptive transport modelling is that further developments and testing are required. Research activities have been initiated to investigate data needs and possible methodologies for incorporating process-based sorption models in the site descriptive modelling.

8 Interactions and integrated modelling

As described in Chapter 2 (Table 2-2), the transport properties modelling uses data and models from other disciplines, and also contributes to the modelling performed within other disciplines. Furthermore, the transport modelling teams will contribute to integrated modelling activities, primarily the development of a geoscientific understanding of the sites and the overall confidence assessment. In this chapter, some suggestions and guidelines for performing this work are given.

8.1 Contributions to other descriptive models

Interactions, in the form of data exchanges, between Transport and other modelling disciplines are described in Chapters 2 through 4. In particular, the input data received from Geology, Hydrogeology and Hydrogeochemistry are described in some detail in Sections 3.2.2, 3.3.2 and 3.4.2, respectively. In this section, the focus is on the use of outputs from Transport in other disciplines, especially the practical aspects of these interactions.

Essentially, the contributions may consist of parameter values and different types of “soft” data that support interpretations made in the process of model development. The parameters could be Primary Data, parameter values interpreted from Primary Data, or estimates based on “expert judgment”. Whereas retardation parameters generally can be expected to be of limited interest to the other disciplines, parameters that describe advection will be used by others, especially Hydrogeology. In particular, some of the methods handled by Transport, primarily tracer tests and groundwater flow measurements, could assist in the parametrisation of hydrogeological models. However, given the limited amount of site-specific data that will be available from these methods, “expert judgment” will be important for assigning advection (and dispersion) parameters.

Tracer tests could also be an important source to “soft” data, especially for investigating the connectivity of the fracture network. Ideally, the characteristic features and properties of the conductive structures should be investigated by a joint effort comprising, e.g. fracture mapping by geological methods, flow logging, single- and multi-well tracer tests, and hydrogeochemical measurements. However, practical restrictions to the use of tracer tests in connection with other characterisation methods could limit their application.

Detailed plans for the needs of transport parameters within other modelling disciplines have not been developed. Rather than attempting to specify these needs (see also Section 4.7), we emphasise the importance of communication and information exchange to secure the access to relevant data and internal and external expertise in the modelling process. In particular, contacts with the site investigation organisations regarding on-going and planned activities (also within other disciplines than Transport), and meetings and other contacts within the site modelling teams are important for such communication.

8.2 Transport parameters of the regolith

The present report is focused on the transport parameters of the rock. However, transport parameters of the regolith, that is, for the different soil units at the investigated sites, are also needed in the site descriptions. These parameters could include parameters that describe various properties of solid phases (soil materials), as well as properties of flow paths (groundwater and/or surface water). In particular, the biosphere modelling within SA requires transport parameters that describe water residence (or turnover) times and distribution coefficients for sorption. There may also be a need for more detailed transport models for investigating specific issues related to site understanding within the site descriptive modelling work, e.g. flow and transport paths between rock and discharge areas at the ground surface.

The strategy for handling the transport modelling and parameters associated with the regolith has not been finally decided. However, a framework for integrated description of the geological, hydrological and hydrogeological properties of the regolith is currently under development within the site modelling teams. To what extent this framework will involve transport parameters has yet to be determined.

Thus, the details of roles, responsibilities and necessary interactions are being discussed at present. Clearly, the physical connection between transport in rock and regolith (the flow paths in the rock discharge into and continue in the regolith), and the fact that similar parameters are to be determined (e.g. sorption parameters), calls for interactions between these two transport modelling activities.

8.3 Development of geoscientific understanding

The development of a geoscientific understanding of the investigated sites is an important part of the site descriptive modelling. This development involves both discipline-specific and integrated aspects. Data and data evaluations of importance for the site understanding of the transport processes are described in Section 7.9. In a broad sense, the main components of the geoscientific understanding associated with the transport processes are to:

- identify and describe the different types of structures that are important for radionuclide transport,
- understand the relative importance of different types of structures, and different geological materials within the structures and the rock matrix,
- understand how the geological, hydrogeological and hydrogeochemical conditions affect the transport processes, and the implications of future changes in these conditions,
- understand how spatial variability affects the transport processes,
- identify the main time scales of the advection and retention processes,
- understand the time dependence of retention, and the limiting factors for the effect of the retention processes.

These different factors or features of the investigated systems should be addressed in the descriptive transport model. Descriptions of site understanding are essentially qualitative. It is important to note that such descriptions will be produced, thereby providing background and support to the numerical parameters in the presented transport models.

Among the investigation methods handled by Transport, tracer tests and groundwater flow measurements have the largest potential for contributing to a more general understanding of the site conditions. As briefly discussed in Section 8.1, the understanding of the conductive structures could be developed through a joint application of methods from different disciplines. In particular, the understanding of the flow and transport properties of more complex structures needs to be developed.

Tracer tests, primarily with non-sorbing and weakly sorbing tracers, could also be an important method for investigating specific structures (fracture zones) at a site. Such investigations could be initiated by the site investigation organisations or within the modelling teams (primarily by Hydrogeology or Transport). Communication within and between these groups is essential for identifying such investigation needs, and to ensure that the tests are planned and carried out so that they provide optimal input to the modelling.

8.4 Contributions to the overall confidence assessment

For reasons discussed in Section 7.9.2, it is anticipated that the contributions from the transport modelling to the overall confidence assessment will be limited. Except for the discipline-specific checks of data and data sources, and an assessment of whether the relevant uncertainties have been described, the main activity related to the judgment of confidence is to analyse the consistency between the transport description and other descriptive models.

Since the geological, hydrogeological and hydrogeochemical descriptions are used as a basis for the transport modelling, consistency is to large extent assured by the modelling process. However, the consistency between the geological characterisation of the samples used in laboratory measurements and the geological description should be checked. If in situ measurements of retardation parameters are carried out, these may give additional support to the identification of different geological units. It is also important to evaluate whether identified needs for additional measurements coincide for the different disciplines, such that, for example, several disciplines would need an additional borehole in a certain geological unit.

9 References

Andersson J, 1999. SR 97. Data and data uncertainties. Compilation of data and data uncertainties for radionuclide transport calculations. SKB TR-99-09. Svensk Kärnbränslehantering AB, Stockholm.

Andersson J, 2003. Site descriptive modelling – strategy for integrated evaluation. SKB R-03-05, Svensk Kärnbränslehantering AB, Stockholm.

Andersson J, Hermanson J, Elert M, Gylling B, Moreno L, Selroos J-O, 1998a. Derivation and treatment of the flow wetted surface and other geosphere parameters in the transport models FARF31 and COMP23 for use in safety assessment. SKB R-98-60. Svensk Kärnbränslehantering AB, Stockholm.

Andersson J, Almén K-E, Ericsson L O, Fredriksson A, Karlsson F, Stanfors R, Ström A, 1998b. Parameters of importance to determine during geoscientific site investigations. SKB TR-98-02. Svensk Kärnbränslehantering AB.

Andersson J, Ström A, Svemar C, Almén K-E, Ericsson L O, 2000. What requirements does the KBS-3 make on the host rock? Geoscientific suitability indicators and criteria for siting and site evaluation. SKB TR-00-12. Svensk Kärnbränslehantering AB, Stockholm.

Andersson J, Berglund J, Follin S, Hakami E, Halvarson J, Hermanson J, Laaksoharju M, Rhén I, Wahlgren C-H, 2002a. Testing the methodology for site descriptive modelling. Application for the Laxemar area. SKB TR-02-19. Svensk Kärnbränslehantering AB, Stockholm.

Andersson J, Christiansson R, Hudson J, 2002b. Site investigations. Strategy for rock mechanics site descriptive model. SKB-TR-02-01. Svensk Kärnbränslehantering AB, Stockholm.

Andersson P, Byegård J, Dershowitz B, Doe T, Hermanson J, Meier P, Tullborg E-L, Winberg A (ed), 2002c. Final report of the TRUE Block Scale project. 1. Characterisation and model development. SKB TR-02-13. Svensk Kärnbränslehantering AB, Stockholm.

Andersson P, Byegård J, Winberg A, 2002d. Final report of the TRUE Block Scale project. 2. Tracer tests in the blockscale. SKB TR-02-14. Svensk Kärnbränslehantering AB, Stockholm.

Birgersson L, Neretnieks I, 1990. Diffusion in the matrix of granitic rock: Field test in the Stripa mine. Water Resour. Res., vol. 26, pp. 2833-2842.

Bodin J, Delay F, de Marsily G, 2003a. Solute transport in a single fracture with negligible matrix permeability: 1. fundamental mechanisms. Hydrogeology J., vol. 11(4), pp. 418-433.

Bodin J, Delay F, de Marsily G, 2003b. Solute transport in a single fracture with negligible matrix permeability: 2. mathematical formalism. Hydrogeology J., vol. 11(4), pp. 434-454.

Bossart P, Hermanson J, Mazurek M, 2001. Äspö Hard Rock Laboratory. Analysis of fracture networks based on the integration of structural and hydrogeological observations on different scales. SKB TR-01-21. Svensk Kärnbränslehantering AB, Stockholm.

Bruno J, de Pablo J, Duro L, Figuerola E, 1995. Experimental study and modelling of the U(VI)-Fe$(OH)_3$ surface precipitation/coprecipitation equilibria. Geochim. Cosmochim. Acta, vol. 59, pp. 4113-4123.

Bruno J, Duro L, de Pablo J, Casas I, Ayora C, Delgado J, Gimeno M J, Pena J, Linklater C, Perez del Villar L., Gómes P, 1998. Estimation of the concentration of trace metals in natural systems. The application of codissolution and coprecipitation approaches to El Berrocal (Spain) and Pocos de Caldas (Brazil). Chem. Geol., vol. 151, pp. 277-291.

Bruno J, Duro L, Grivé M, 2001. The applicability and limitations of thermodynamic geochemical models and tools used in simulating radionuclide behaviour in natural waters. Lessons learned from the Blind Predictive Modelling exercises performed in conjunction with Natural Analogue studies. SKB TR-01-20. Svensk Kärnbränslehantering AB, Stockholm.

Bruno J, Duro L, Grivé M, 2002. The applicability and limitations of thermodynamic geochemical models to simulate trace element behaviour in natural waters. Lessons learned from natural analogue studies. Chem. Geol., vol. 190, pp. 371-393.

Byegård J, Johansson H, Skålberg M, Tullborg E-L, 1998. The interaction of sorbing and non-sorbing tracers with different Äspö rock types. Sorption and diffusion experiments in the laboratory scale. SKB TR-98-18. Svensk Kärnbränslehantering AB, Stockholm.

Byegård J, Johansson H, Andersson P, Hansson K, Winberg A, 1999. Äspö Hard Rock Laboratory. Test plan for the long term diffusion experiment. SKB IPR-99-36. Svensk Kärnbränslehantering AB, Stockholm.

Carbol P, Engkvist I, 1997. Compilation of radionuclide sorption coefficients for performance assessment. SKB R-97-13. Svensk Kärnbränslehantering AB, Stockholm.

Cheng H, Cvetkovic V, Selroos J O, 2003. Hydrodynamic control of tracer retention in heterogeneous rock fractures. Water Resour. Res., 39(5), 1130, doi:10.1029/2002WR001354.

Cvetkovic V, 2003. Potential impact of colloids on plutonium migration at the Äspö site. SKB R-03-16. Svensk Kärnbränslehantering AB, Stockholm.

Cvetkovic V, Cheng H, 2002. Äspö Hard Rock Laboratory. TRUE Block Scale project. Evaluation of block scale tracer retention understanding experiments at Äspö HRL. SKB IPR-02-33. Svensk Kärnbränslehantering AB, Stockholm.

Cvetkovic V, Selroos J-O, Cheng H, 1999. Transport of reactive tracers in rock fractures. J. Fluid Mech., vol. 378, pp. 335-356.

Cvetkovic V, Cheng H, Selroos J-O, 2000. First TRUE stage. Evaluation of Tracer Retention Understanding Experiments (first stage) at Äspö. SKB ICR-00-01. Svensk Kärnbränslehantering AB, Stockholm.

Cvetkovic V, Painter S, Outters N, Selroos J O, 2004. Stochastic simulation of radionuclide migration in discretely fractured rock near the Äspö Hard Rock Laboratory. Water Resour. Res., 40, WR02404, doi:10.1029/2003WR002655.

Dershowitz W, Lee G, Geijer J, Foxford T, LaPoint P, Thomas A, 1995. FRACMAN – Interactive discrete feature data analysis, geometric modelling and exploration simulation. User documentation, version 2.5. Golder Associates Inc.

Dershowitz W, Eiben T, Follin S, Andersson J, 1999. SR 97 – Alternative models project. Discrete fracture network modelling for performance assessment of Aberg. SKB R-99-43. Svensk Kärnbränslehantering AB.

Dershowitz B, Winberg A, Hermanson J, Byegård J, Tullborg E-L, Andersson P, Mazurek M, 2003. Äspö Task Force. Task 6C. A semi-synthetic model of block scale conductive structures at the Äspö Hard Rock Laboratory. SKB IPR-03-13. Svensk Kärnbränslehantering AB.

Elert M, Svensson H, 2001. Evaluation of modelling of the TRUE-1 radially converging tests with sorbing tracers. The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. SKB TR-01-12. Svensk Kärnbränslehantering AB, Stockholm.

Gustafsson E, 2002. Beräkning av grundvattenflödet i en sprickzon med hjälp av utspädningsteknik, en metodstudie. SKB R-02-30. Svensk Kärnbränslehantering AB, Stockholm. (In Swedish)

Gylling B, 1997. Development and applications of the Channel Network model for simulations of flow and solute transport in fractured rock. Ph.D. Thesis, Department of Chemical Engineering and Technology, Royal Institute of Technology (KTH), Stockholm.

Gylling B, Moreno L, Neretnieks I, 1999. SR 97 – Alternative models project. Channel network modelling of Aberg. Performance assessment using CHAN3D. SKB R-99-44. Svensk Kärnbränslehantering AB.

Hartley L J, Holton D, 2003. CONNECTFLOW (Release 2.0) Technical Summary Document. SERCO/ERRA-C/TSD02V1, CONNECTFLOW Homepage: http://www.sercoassurance.com/ea/groundwater/conflow.htm.

Hartley L J, Holton D, Hoch A R, 2003a. NAPSAC (Release 4.4) Technical Summary Document. SERCO/ERRA-N/TSD02V1, CONNECTFLOW Homepage: http://www.sercoassurance.com/ea/groundwater/conflow.htm.

Hartley L J, Hoch A R, Cliffe K A C, Jackson C P, Holton D, 2003b. NAMMU (Release 7.2) Technical Summary Document. SERCO/ERRA-NM/TSD02V1, CONNECTFLOW Homepage: http://www.sercoassurance.com/ea/groundwater/conflow.htm.

Hedin A, 2001. Integrated analytic radionuclide transport model for spent nuclear fuel repository in saturated fractured rock. Nuclear Technology, vol. 138, pp. 179-205.

Holmén J G, 1997. On the flow of groundwater in closed tunnels: Generic hydrogeologic modelling of nuclear waste repository SFL 3-5. Ph.D. Thesis, Department of Earth Sciences, Uppsala University, Uppsala.

Jakob A, Mazurek M, Heer W, 2003. Solute transport in crystalline rocks at Äspö – II: Blind predictions, inverse modelling and lessons learnt from test STT1. J. Contam. Hydrol., vol. 61, pp. 175-190.

Kersting A B, Efurd D W, Finnegan D L, Rokop D J, Smith D K, Thompson J L, 1999. Migration of plutonium in ground water at the Nevada Test Site. Nature, vol. 397, pp. 56-59.

Klos R A, White M J, Wickham S M, Bennett D G, Hicks T W, 2002. Quantitative assessment of the potential significance of colloids to the KBS-3 disposal concept. SKI Report 02:34. Statens Kärnkraftinspektion, Stockholm.

Laaksoharju M, Skårman C, Skårman E, 1999. Multivariate Mixing and Mass balance (M3) calculations: A new tool for decoding hydrogeochemical information. Appl. Geochem., vol. 14, pp. 861-871.

Landström O, Tullborg E-L, Eriksson G, Sandell Y, 2001. Effects of glacial/post-glacial weathering compared with hydrothermal alteration – implications for matrix diffusion. Results from drillcore studies in porphyritic quartz monzodiorite from Äspö SE Sweden. SKB R-01-37. Svensk Kärnbränslehantering AB, Stockholm.

Lee H S, Moreno L, Neretnieks I, 1990. Some properties of a channel network model. In Proceedings from Geoval-1990, Symposium on Validation of Geoshere Flow and Transport Models, Organised by the Swedish Nuclear Power Inspectorate (SKI) and the OECD/NEA, Stockholm, 14-17 May 1990.

Lindgren M, Gylling B, Elert M, 2002. FARF31 Version 1.2. User's guide. SKB TS-02-03. Svensk Kärnbränslehantering AB, Stockholm.

Löfgren A, Brydsten L, Engkvist A, Lindborg T, Lundin L, 2003. Ecological site descriptive model – a strategy for the development during site investigations. SKB R-03-06. Svensk Kärnbränslehantering AB, Stockholm.

Löfgren M, Neretnieks I, 2002. Formation factor logging in-situ by electrical methods. Background and methodology. SKB TR-02-27. Svensk Kärnbränslehantering AB, Stockholm.

Löfgren M, Neretnieks I, 2003. Formation factor logging by electrical methods. Comparison of formation factor logs obtained in situ and in the laboratory. J. Contam. Hydrol., vol. 61, pp. 107-115.

Malmström M, 2004. Personal communication.

Malmström M E, Destouni G, Martinet P, 2004. Modelling expected solute concentration in randomly heterogeneous flow systems with multi-component reactions. Env. Sci. Technol., in press.

Mazurek M, Bossart P, Eliasson T, 1997. Classification and characterisation of water-conducting features at Äspö: Results of investigations at the outcrop scale. SKB ICR-97-01. Svensk Kärnbränslehantering AB, Stockholm.

Mazurek M, Jakob A, Bossart P, 2003. Solute transport in crystalline rocks at Äspö – I: Geological basis and model calibration. J. Contam. Hydrol., vol. 61, pp. 157-174.

Munier R, Hermanson J, 2001. Metodik för geometrisk modellering. Presentation och administration av platsbeskrivande modeller. SKB R-01-15. Svensk Kärnbränslehantering AB, Stockholm. (In Swedish)

Munier R, Stenberg L, Stanfors R, Milnes A G, Hermanson J, Triumf C-A, 2003. Geological site descriptive model – a strategy for the model development during site investigations. SKB R-03-07. Svensk Kärnbränslehantering AB, Stockholm.

Möri A, Mazurek M, Adler M, Schild M, Siegesmund S, Vollbrecht A, Ota K, Ando T, Alexander W R, Smith P A, Haag P, Bühler C, 2003. The Nagra-JNC in situ study of safety relevant radionuclide retardation in fractured crystalline rock. IV: The in situ study of matrix porosity in the vicinity of a water conducting fracture. Nagra Technical Report 00-08. Nagra, Wettingen, Switzerland.

NEA (Nuclear Energy Agency), 2001. Using thermodynamic sorption models for guiding radioelement distribution coefficient (K_d) investigations. A status report. ISBN 92-64-18679-4, NEA, Paris, France.

Neretnieks I, 1980. Diffusion in the rock matrix: An important factor in radionuclide retardation? J. Geophys. Res., vol. 85, no. B8, pp. 4379-4397.

Neretnieks I, 2002. A stochastic multi-channel model for solute transport – analysis of tracer test in fractured rock. J. Contam. Hydrol., vol. 55, pp. 175-211.

Neretnieks I, Moreno L, 2003. Prediction of some in situ tracer tests with sorbing tracers using independent data. J. Contam. Hydrol., vol. 61, pp. 351-360.

Norman S, 1992. HYDRASTAR – A code for stochastic simulation of groundwater flow. SKB TR-92-12. Svensk Kärnbränslehantering AB, Stockholm.

Norman S, Kjellbert N, 1990. FARF31 – A far field radionuclide migration code for use with the PROPER package. SKB TR-90-01. Svensk Kärnbränslehantering AB, Stockholm.

Nordqvist R, Gustafsson E, 2002. Single-well injection-withdrawal tests (SWIW). Literature review and scoping calculations for homogeneous crystalline bedrock conditions. SKB R-02-34. Svensk Kärnbränslehantering AB, Stockholm.

Ohlsson Y, 2000. Studies of ionic diffusion in crystalline rock. Ph.D. Thesis, Department of Chemical Engineering and Technology, Royal Institute of Technology (KTH), Stockholm.

Ohlsson Y, Neretnieks I, 1997. Diffusion data in granite. Recommended values. SKB TR-97-20. Svensk Kärnbränslehantering AB, Stockholm.

Parkhurst, D L, Appelo C A J, 1999. User's guide to PHREEQC (version 2). USGS Water-Resources Investigations Report 99-4259, United States Geological Survey, Denver, Colorado, USA.

Poteri A, Billaux D, Dershowitz W, Gomez-Hernandez JJ, Cvetkovic V, Hautojärvi A, Holton D, Medina A, Winberg A (ed), 2002. Final report of the TRUE Block Scale project. 3. Modelling of flow and transport. SKB TR-02-15. Svensk Kärnbränslehantering AB, Stockholm.

Rhén I, Follin S, Hermanson J, 2003. Hydrogeological site descriptive model – a strategy for the development during site investigations. SKB R-03-08. Svensk Kärnbränslehantering AB, Stockholm.

Romero L, Thompson A, Moreno L, Neretnieks I, Widén H, Boghammar A, 1999. Comp23/Nuctran user's guide. Proper version 1.1.6. SKB R-99-64. Svensk Kärnbränslehantering AB, Stockholm.

Saksa P, Nummela J, 1998. Geological-structural models used in SR 97. Uncertainty analysis. SKB TR-98-12. Svensk Kärnbränslehantering AB, Stockholm.

Selroos J-O, Walker D D, Ström A, Gylling B, Follin S, 2002. Comparison of alternative modelling approaches for flow and transport in fractured rock. J. Hydrology, vol. 257, pp. 174-188.

SKB, 1999a. Deep repository for spent nuclear fuel. SR 97 – Post-closure safety. Main report – Vol. I, Vol. II and Summary. SKB TR-99-06. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 1999b. SR 97. Processes in the repository evolution. Background report to SR 97. SKB TR-99-07. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 2000. Geoscientific programme for investigation and evaluation of sites for the deep repository. SKB TR-00-20. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 2001a. Integrated account of method, site selection and programme prior to the site investigation phase. SKB TR-01-03. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 2001b. Site investigations. Investigation methods and general execution programme. SKB TR-01-29. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 2001c. Feasibility studies – Östhammar, Nyköping, Oskarshamn, Tierp, Hultsfred and Älvkarleby. Summary report. SKB TR-01-16. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 2002a. Forsmark – site descriptive model version 0. SKB R-02-32. Svensk Kärnbränslehantering AB, Stockholm.

SKB, 2002b. Simpevarp – site descriptive model version 0. SKB R-02-35. Svensk Kärnbränslehantering AB, Stockholm.

Smellie J, Laaksoharju M, Tullborg E-L, 2002. Hydrogeochemical site descriptive model – a strategy for the model development during site investigations. SKB R-02-49. Svensk Kärnbränslehantering AB, Stockholm.

Sundberg J, 2003. Thermal site descriptive model – a strategy for the model development during site investigations. SKB R-03-10. Svensk Kärnbränslehantering AB, Stockholm.

Svensson, U., 2004. DarcyTools V2.1. Verification and validation, SKB R-04-21. Svensk Kärnbränslehantering AB, Stockholm.

Svensson, U., Ferry, M., 2004. DarcyTools V2.1. User's Guide, SKB R-04-20. Svensk Kärnbränslehantering AB, Stockholm.

Svensson, U., Kuylenstierna, H-O., Ferry, M., 2004. DarcyTools V2.1. Concepts, methods, equations and demo simulations, SKB R-04-19. Svensk Kärnbränslehantering AB, Stockholm.

Tukiainen V, 2002. Methods for the streamline calculation and for the estimation of transport resistance in fractures. Working Report 2002-06. Posiva Oy, Helsinki, Finland.

Widén H, Walker D, 1999. SR 97 – Alternative models project. Stochastic continuum modelling of Aberg. SKB R-99-42. Svensk Kärnbränslehantering AB, Stockholm.

Widestrand H, Byegård J, Ohlsson Y, Tullborg E-L, 2003. Strategy for the use of laboratory methods in the site investigations programme for the transport properties of the rock. SKB R-03-20. Svensk Kärnbränslehantering AB, Stockholm.

Winberg A, Andersson P, Hermansson J, Byegård J, Cvetkovic V, Birgersson L, 2000. Äspö Hard Rock Laboratory. Final report on the first stage of the tracer retention understanding experiments. SKB TR-00-07. Svensk Kärnbränslehantering AB, Stockholm.

Winberg A, Andersson P, Byegård J, Poteri A, Cvetkovic V, Dershowitz B, Doe T, Hermanson J, Gomez-Hernandez J-J, Hautojärvi A, Billaux D, Tullborg E-L, Meier P, Medina A, 2002. Final report of the TRUE Block Scale project. 4. Synthesis of flow, transport and retention in the block scale. SKB TR-02-16. Svensk Kärnbränslehantering AB, Stockholm.

Xu S, Wörman A, 1998. Statistical patterns of geochemistry in crystalline rock and effect of sorption kinetics on radionuclide migration. SKI Report 98:41. Statens Kärnkraftinspektion, Stockholm.

Zhu C, 2002. Estimation of surface precipitation constants for sorption of divalent metals onto hydrous ferric oxide and calcite. Chem. Geol., vol. 188, pp. 23-32.

Appendix A

Mathematical modelling and flow-related parameters

In this appendix, mathematical approaches are summarised with the aim to give a background to, and explicit expressions for, the flow-related transport parameters. More comprehensive descriptions of mathematical modelling of solute transport in fractured rock are given by /Bodin et al, 2003/, a general review, /Poteri et al, 2002/ and /Cvetkovic and Cheng, 2002/, concerning the present modelling approach. In addition, /Cheng et al, 2003/ and /Cvetkovic et al, 2004/ presented numerical modelling results for a single fracture and a fracture network, respectively, based on a theory closely related to that described herein.

The basic underlying assumptions are those given in Section 4.3.1. Additionally, we consider a parallel plate model for description of the individual fractures /e.g. Neretnieks, 1980/, and assume complete mixing in the transverse direction within the fracture (across the fracture aperture) and constant values of the diffusion and sorption parameters in the transverse direction within the matrix. Under these assumptions, the general, three-dimensional transport equations for advection, dispersion, and retention of a single solute can be expressed as

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} = \sum_i \psi_1^{(j)} \tag{A-1}$$

$$\frac{\partial C^{*(j)}}{\partial t} = \psi_2^{(j)} \tag{A-2}$$

where Equation A-1 is the mass balance of the mobile zone, with C being the solute concentration and **J** the mass flux vector (includes, in the general case, advection and dispersion). The functions $\psi_1^{(j)}$ and $\psi_2^{(j)}$ define the interactions between the mobile and immobile zones, accounting for multiple immobile zones (index j), each characterised by a concentration C^*. The processes expressed by $\psi_1^{(j)}$ and $\psi_2^{(j)}$ may include diffusion and sorption in different immobile zones, as well as radioactive decay.

Different simplifications of Equations (A-1) and (A-2) can be considered in order to obtain analytical solutions, either in the Laplace domain or in the real domain. The conventional modelling approach is based on a one-dimensional advection-dispersion formulation, often with retention in the form of surface sorption and diffusion and sorption in the matrix (that is, retardation processes only). Neglecting radioactive decay, the transport equations can be written as

$$R_a \frac{\partial C}{\partial t} + V \frac{\partial C}{\partial x} - D_L \frac{\partial^2 C}{\partial x^2} - a_w D_e \left.\frac{\partial C^*}{\partial z}\right|_{z=0} = 0 \tag{A-3}$$

$$R_m \frac{\partial C^*}{\partial t} - \frac{D_e}{\theta_m} \frac{\partial^2 C^*}{\partial z^2} = 0 \tag{A-4}$$

where x is the direction of flow and advective-dispersive transport, z is the direction perpendicular to flow (the direction of matrix diffusion), V is the groundwater velocity, D_L is the longitudinal dispersion coefficient, and a_w [L^{-1}] is the specific surface of the

fractures. The specific surface area quantifies the area available for mass transfer between the mobile and immobile zones; a_w is defined as surface area per unit volume of water. Equilibrium sorption is expressed through two retardation factions; $R_a = 1 + a_w K_a$ for surface sorption, and
$R_m = 1 + \rho K_d / \theta_m$ for sorption in the rock matrix.

It should be noted that the simplified one-dimensional system in Equations (A-3) – (A-4) includes a geometric parameter that quantifies the surface area for mass transfer (we have assumed that the same surface area is applicable to both immobile domains). Analytical solutions can be obtained only in the Laplace domain, see /Hedin, 2001/. In the real domain, analytical solutions are available only if dispersion is neglected /see, e.g. Lee et al, 1990/.

Whereas one-dimensional advection-dispersion approaches frequently have been applied in field-scale "streamtube" modelling of transport /Norman and Kjellbert, 1990/, dispersion-free models are usually not applicable on the field scale in a strictly one-dimensional Cartesian sense. However, the analytical solutions to such equations can be considered mathematically equivalent to the solutions for individual segments along transport paths in trajectory- or transport path-oriented models (cf. below), and can therefore be used in that context.

Equations (A-3) – (A-4) are consistent with a continuum (Eulerian) approach to transport modelling, which, as indicated above, requires rather restrictive geometric assumptions to make analytical solutions possible. More general analytical solutions can obtained with a discrete (Lagrangian) formulation as a starting point. Neglecting dispersion in the three-dimensional system (A-1) – (A-2), and with the same retention processes as in Equations (A-3) – (A-4), a discrete formulation results in the following transport equations /cf. Cvetkovic and Cheng, 2002/:

$$\left(1 + \frac{K_a}{b}\right)\frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C - \frac{D_e}{b}\frac{\partial C^*}{\partial z}\bigg|_{z=0} = 0 \qquad \text{(A-5)}$$

$$R_m \frac{\partial C^*}{\partial t} - \frac{\partial}{\partial z}\frac{D_e}{\theta_m}\frac{\partial C^*}{\partial z} = 0 \qquad \text{(A-6)}$$

In a stochastic description of transport where all parameters may display random spatial variability, this equation system is consistent with a discrete view of transport, either as random trajectories of discrete particles, or as random streamtubes of tracer "parcels" carried by a constant flow rate through a network of fractures. Thus, transport takes place in a three-dimensional flow field, but can be viewed as a one-dimensional transport problem along the particle trajectory or streamtube.

The parameter b [L] in Equations (A-5) – (A-6) is a generalised, spatially variable "half-aperture", which can be interpreted as a characteristic retention scale (essentially, the probability of the particle getting "transferred" to the immobile zones is taken to be inversely proportional to the "mean distance" from the water to the fracture wall). This implies that a parameter of geometric character is required also in the discrete formulation, although it can be given a more general interpretation. Furthermore, it should be noted that z is a generalised transverse co-ordinate, which means that it is transverse to the fracture plane irrespective of the orientation of the plane.

For pulse injection of unit mass, the solution to (A-5) - (A-6) can be expressed as a probability density function for the residence time of a single particle between injection and exit locations in the transport domain /Cvetkovic and Cheng, 2002/

$$\gamma(t,t_w) = \frac{H(t-t_w)B}{2\sqrt{\pi}(t-t_w-A)^{3/2}} \exp\left[\frac{-B^2}{4(t-t_w-A)}\right] \qquad \text{(A-7)}$$

where H is the Heaviside step function, t_w [T] is the water residence time, A [T] is a surface sorption parameter group, and B [$T^{1/2}$] is referred to as “total transport resistance”. In view of the stochastic modelling approach and the one-dimensional description of transport along a three-dimensional trajectory, all of these quantities can be expressed as sums of random components along the trajectory:

$$t_w = \sum_{i=1}^{N} t_{w,i}\ ; \qquad A = \sum_{i=1}^{N} A_i\ ; \qquad B = \sum_{i=1}^{N} B_i \qquad \text{(A-8)}$$

where the index “*i*” denotes either a fracture, if the particle is transported through a series of internally homogeneous fractures, and/or discretisation segments if we consider single or series of heterogeneous fractures; N is the total number of fractures/segments.

If each segment is characterised by a velocity V_i, length l_i, and half-aperture b_i, then the characteristic advection and surface sorption parameters are defined as

$$t_w = \sum_{i=1}^{N} \frac{l_i}{V_i}\ ; \qquad A = \sum_{i=1}^{N} K_{a,i} F_i\ ; \qquad F_i = \frac{l_i}{V_i b_i} = \frac{t_{w,i}}{b_i} \qquad \text{(A-9)}$$

where F_i [TL^{-1}] has been referred to as “hydrodynamic transport resistance” or “transport resistance”; here we denote this parameter group simply as “*F*-parameter”. If diffusion and sorption parameters θ_m, D_e and R_m for the matrix are assumed uniform within fractures (segments), but can vary among segments, then B can be expressed as

$$B = \sum_{i=1}^{N} M_i F_i\ ;\ M_i = \sqrt{\theta_{m,i} D_{e,i} R_{m,i}} = \sqrt{\theta_{m,i} D_{e,i}\left(1 + \frac{K_{d,i}\rho}{\theta_{m,i}}\right)} \qquad \text{(A-10)}$$

where M_i is referred to as “material parameters group”. In cases where different discretisations/resolutions are used for describing, for instance, advection and retardation parameters, index “*i*” refers to the smallest scale of resolution.

If the retardation parameters are uniform (constant) in the entire domain, then

$$A = K_a F\ ;\ \ B = M\,F\ ;\ \ M = \sqrt{\theta_m D_e R_m} = \sqrt{\theta_m D_e\left(1 + \frac{K_d \rho}{\theta_m}\right)}\ ;\ \ F = \sum_{i=1}^{N} F_i \qquad \text{(A-11)}$$

which implies that only t_w and F need to be obtained by integration along the trajectory, and that only the integrated “*F*-parameter” is required (not the integrated product of F_i and some other parameter).

Note that many different formulations of the “materials parameter group” have been presented in the literature. In principle, all parameters in the group (porosity, diffusivity, density and sorption parameters) can be defined in different ways, which implies that a multitude of expressions for the group can be obtained. Furthermore, for strongly sorbing solutes, M^i in (A-10) can be simplified as

$$M_i = \sqrt{\theta_{m,i} D_{e,i} \left(1 + \frac{K_{d,i}\rho}{\theta_{m,i}} \right)} \approx \sqrt{D_{e,i} K_{d,i} \rho} \qquad \text{(A-12)}$$

which is independent of the matrix porosity. Similarly, the "retarded travel time", in the solution (A-7) can be simplified as $t_w + A \approx A$ for strongly sorbing solutes /Andersson et al, 1998b/.

Eqs (A-9) – (A-11) presents characteristic parameter groups that provide a complete description of solute transport in a heterogeneous fractured medium. In particular, if transport is viewed as consisting of solute particles following random trajectories through a fracture network, the "F-parameter" associated with a given trajectory can be quantified by integrating $t_{w,i} / b_i$ for the different fractures or segments along the trajectory. However, in some cases other parameters for the segments are more readily available. In particular, DFN models often provide a description in terms of flow rate and geometric parameters for the individual segments. Focusing on the hydrodynamic parameters and a description of the transport path as a series of segments or "sub-paths" of widths W_i (width in the fracture plane, perpendicular to the flow direction) half-apertures b_i and volumetric flow rates, Q_i, the following expressions are obtained:

$$t_w = 2\sum_{i=1}^{N} \frac{W_i l_i b_i}{Q_i}\,; \qquad F = 2\sum_{i=1}^{N} \frac{W_i l_i}{Q_i} \qquad \text{(A-13)}$$

where the product 2 $W_i\, l_i$ defines an area for each segment, over which the solute is in contact with the rock matrix; note, however, that the quotient $W_i l_i / Q_i$ should be integrated, not the individual parameters.

If solute transport is viewed as taking place along a streamtube with a given flow rate, then the travel time and "*F*-parameter" can be written as

$$t_w = \frac{2}{Q}\sum_{i=1}^{N} W_i l_i b_i\,; \qquad F = \frac{2}{Q}\sum_{i=1}^{N} W_i l_i \qquad \text{(A-14)}$$

where $2\,\Sigma\, W_i\, l_i b_i$ and $2\,\Sigma\, W_i\, l_i$ define the total volume and contact area, respectively, for the streamtube. Thus, different descriptions are associated with different characteristic parameter groups. For any basic description, a consistent treatment of the characteristic parameter groups is required for a correct quantification of field-scale transport.

Finally, it should be noted that Cvetkovic and co-workers /e.g. Cvetkovic et al, 2000; Cvetkovic and Cheng, 2002/ use a different notation for the flow-related parameters. In the equations presented above, which essentially are taken from their works, we have replaced their parameters τ and β by t_w and F, respectively. This is done to facilitate comparisons with previous Safety Assessments (primarily SR 97), and for consistency with the general programme for the Site Investigations.

References

Bodin J, Delay F, de Marsily G, 2003. Solute transport in a single fracture with negligible matrix permeability: 2. mathematical formalism. Hydrogeology J., vol. 11(4), pp. 434-454.

Cheng H, Cvetkovic V, Selroos J O, 2003. Hydrodynamic control of tracer retention in heterogeneous rock fractures. Water Resour. Res., 39(5), 1130, doi:10.1029/2002WR001354.

Cvetkovic V, Cheng H, 2002. Äspö Hard Rock Laboratory. TRUE Block Scale project. Evaluation of block scale tracer retention understanding experiments at Äspö HRL. SKB IPR-02-33. Svensk Kärnbränslehantering AB, Stockholm.

Cvetkovic V, Cheng H, Selroos J-O, 2000. First TRUE stage. Evaluation of Tracer Retention Understanding Experiments (first stage) at Äspö. SKB ICR-00-01. Svensk Kärnbränslehantering AB, Stockholm.

Cvetkovic V, Painter S, Outters N, Selroos J O, 2004. Stochastic simulation of radionuclide migration in discretely fractured rock near the Äspö Hard Rock Laboratory. Water Resour. Res., 40, WR02404, doi:10.1029/2003WR002655.

Hedin A, 2001. Integrated analytic radionuclide transport model for spent nuclear fuel repository in saturated fractured rock. Nuclear Technology, vol. 138, pp. 179-205.

Lee H S, Moreno L, Neretnieks I, 1990. Some properties of a channel network model. In Proceedings from Geoval-1990, Symposium on Validation of Geoshere Flow and Transport Models, Organised by the Swedish Nuclear Power Inspectorate (SKI) and the OECD/NEA, Stockholm, 14-17 May 1990.

Neretnieks I, 1980. Diffusion in the rock matrix: An important factor in radionuclide retardation? J. Geophys. Res., vol. 85, no. B8, pp. 4379-4397.

Poteri A, Billaux D, Dershowitz W, Gomez-Hernandez JJ, Cvetkovic V, Hautojärvi A, Holton D, Medina A, Winberg A (ed), 2002. Final report of the TRUE Block Scale project. 3. Modelling of flow and transport. SKB TR-02-15. Svensk Kärnbränslehantering AB, Stockholm.