

R-03-05

Site descriptive modelling – strategy for integrated evaluation

Johan Andersson, JA Streamflow AB

February 2003

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



Site descriptive modelling – strategy for integrated evaluation

Johan Andersson, JA Streamflow AB

February 2003

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

A pdf-version of this document can be downloaded from www.skb.se

Abstract

The current document establishes the strategy to be used for achieving sufficient integration between disciplines in producing Site Descriptive Models during the Site Investigation stage. The Site Descriptive Model should be a multidisciplinary interpretation of geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties and ecosystems using site investigation data from deep bore holes and from the surface as input. The modelling comprise the following iterative steps, evaluation of primary data, descriptive and quantitative modelling (in 3D), overall confidence evaluation.

Data are first evaluated within each discipline and then the evaluations are checked between the disciplines. Three-dimensional modelling (i.e. estimating the distribution of parameter values in space and its uncertainty) is made in a sequence, where the geometrical framework is taken from the geological model and in turn used by the rock mechanics, thermal and hydrogeological modelling etc. The three-dimensional description should present the parameters with their spatial variability over a relevant and specified scale, with the uncertainty included in this description. Different alternative descriptions may be required.

After the individual discipline modelling and uncertainty assessment a phase of overall confidence evaluation follows. Relevant parts of the different modelling teams assess the suggested uncertainties and evaluate the feedback. These discussions should assess overall confidence by, checking that all relevant data are used, checking that information in past model versions is considered, checking that the different kinds of uncertainty are addressed, checking if suggested alternatives make sense and if there is potential for additional alternatives, and by discussing, if appropriate, how additional measurements (i.e. more data) would affect confidence.

The findings as well as the modelling results are to be documented in a Site Description. This description encompasses the different databases and digital models developed as well as a model report with associated sub-documentation. The model report should not only present the models, but also how they were derived. Model reports for different sites should follow the same outline.

Summary

Development of Site Descriptive Models is an essential part of the Site Investigations carried out by the Swedish Nuclear Fuel and Waste Management Company (SKB). The current document establishes the strategy to be used for achieving sufficient integration between disciplines in this modelling. The strategy for integrated evaluation as described in the current document is not a strict and detailed instruction for how to carry out such a complex task. It provides a basic structure to the modelling process, it discusses issues and suggests means of addressing issues. Clearly, during the course of the modelling work challenges not anticipated here will arise and be resolved. The entire modelling process will be a learning process and the modelling strategy must be flexible and updated accordingly.

Modelling steps

The Site Descriptive Model should be a multidisciplinary interpretation of geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties and ecosystems using site investigations from deep bore holes and from the surface as input. The modelling comprise the following iterative steps:

- Evaluation of primary data.
- Descriptive and quantitative modelling (in 3D).
- Overall confidence evaluation.

The measured (primary) data constitute a wide range of different measurement results. These data both need to be checked for consistency and to be interpreted into a format more amenable for three-dimensional modelling. Examples of such evaluations are estimation of surface geology, lineament interpretation, geological single hole interpretation, assessment of reflection seismics, hydrogeological single hole interpretation, assessment of hydrogeochemical data and single hole assessment of rock stress measurements. The data are first evaluated within each discipline and then the evaluations are checked between the disciplines.

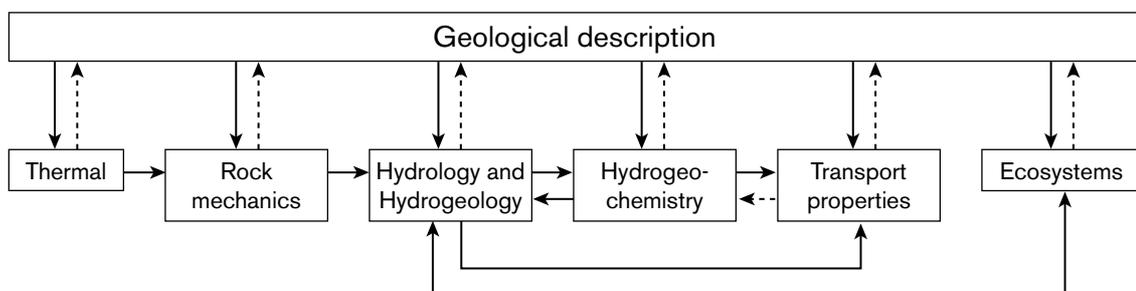


Figure 1. The different discipline descriptions are interrelated with several feedback loops and where geology provides the essential geometrical framework.

The actual three-dimensional modelling (i.e. estimating the distribution of parameter values in space) is made in a sequence where the geometrical framework is taken from the geological model and in turn used by the rock mechanics, thermal and hydrogeological modelling. The hydrogeochemical description is to some extent developed independently, but its consistency with the hydrogeological description is checked. The description of transport properties is based on the hydrogeological and hydrogeochemical descriptions, although additional data are assessed as well. Finally, the description of the near surface is made essentially independent of the other descriptions, but the interface between geosphere and biosphere is handled jointly with (essentially) hydrogeology. Even if most of these first steps in the development chain are made within each discipline the other disciplines should be kept sufficiently informed, e.g. through the project group meetings, on the progress of these evaluations.

After the individual discipline modelling and uncertainty assessment a phase of overall confidence evaluation follows. Relevant parts of the different modelling teams assess the suggested uncertainties and evaluate the feedback, in particular to the suggested geology, hydrogeology and hydrogeochemistry description. After revisions the teams re-assess the model description with its uncertainty and confidence statements. These discussions should assess overall confidence by:

- checking that all relevant data are used,
- checking that information in past model versions is considered,
- checking that the different kinds of uncertainty listed in chapter 4 are addressed,
- checking if suggested alternatives make sense and if there is potential for additional alternatives,
- and by discussing, if appropriate, how additional measurements (i.e. more data) would affect confidence.

Assessment of uncertainty and confidence

There are always uncertainties in interpreting measurements and rock parameters, which vary in space. The three-dimensional description should present the parameters with their spatial variability over a relevant and specified scale, with the uncertainty included in this description. Different alternative descriptions may be required. In addition, it is also necessary to describe the confidence in the model predictions.

There are several challenges, which needs to be handled when dealing with alternatives. In particular, it may be difficult for modelling teams to develop different alternative models in parallel. Furthermore, as models are used as input to the other models the total number of alternatives may become impractical to handle – ‘variant explosion’. Alternative generation should be seen as a means for model development in general and as a means of exploring the confidence. All alternatives need not be equally probable. Different alternatives should focus on clear differences in the geometrical framework and on clear differences on the description of the rock properties.

The confidence in the descriptive model is essentially a qualitative entity. Still, judgement of confidence needs to be based on several quantitative analyses. For example:

- The method of interpretation is key to the confidence assessment. A similar and unbiased treatment of all different data and interpretations that explains several different observations enhances confidence.
- Consistency (i.e. no conflicts) between the different discipline model interpretations and with the geological evolution model enhances confidence.
- Data and data sources need to be quality assured according to issued manuals and procedures. Yet, this is a necessary but not a sufficient condition for confidence – the data also need to be properly understood! Also the users need to check the input data.
- Small estimated uncertainties and inability to produce many different alternative interpretations from the same database are indications of confidence – although no strict proof.
- If analyses by an additional team(s) lead to similar conclusions.
- Another indication of confidence is to what extent measurement results from late stages of the investigation compare well with previous predictions.

The latter point will also be important for discussing the potential benefit of additional measurements. Clearly, if new data compare well with the previous prediction, the need for yet additional data may diminish.

Documentation

The findings as well as the modelling results are to be documented in a Site Description. This description encompasses the different databases and digital models developed as well as a model report with associated supporting documentation. It is essential that the model report covers the following:

- References to data sources and identification of previous model versions.
- Means of primary data evaluation including; the disciplinary evaluation, re-evaluation of previously evaluated data and means of interdisciplinary comparisons.
- Means of three dimensional modelling including the disciplinary evaluation with its comparisons with previous model versions, uncertainty estimates and the joint uncertainty and confidence evaluation.
- Presentation of the Site Descriptive Model (discipline by discipline) with its uncertainties and alternatives.
- Comparison with previous model versions, assessment on overall confidence and discussing potentially fruitful additions to the measurement programme.

Model reports for different sites should have the same table of contents.

Contents

| | | |
|----------|--|----|
| 1 | Introduction | 11 |
| 1.1 | Requirements | 11 |
| 1.2 | Approach to developing the strategy | 12 |
| 1.3 | This report | 12 |
| 2 | Site Descriptive Modelling | 13 |
| 2.1 | Overview | 13 |
| 2.2 | Organisational setup | 14 |
| 2.3 | Evaluation of primary data | 15 |
| 2.3.1 | Assembling primary data | 15 |
| 2.3.2 | Evaluating primary data within each discipline | 15 |
| 2.3.3 | Interdisciplinary comparisons | 17 |
| 2.4 | Descriptive modelling in 3D | 17 |
| 2.4.1 | Selecting the model domain | 18 |
| 2.4.2 | Estimating structures and properties in three dimensions | 18 |
| 2.5 | Overall evaluation of confidence | 23 |
| 2.6 | Documentation | 25 |
| 2.6.1 | Digital information | 25 |
| 2.6.2 | The model report | 25 |
| 3 | Assessment of uncertainty and confidence | 27 |
| 3.1 | Definitions | 27 |
| 3.1.1 | Scenario uncertainty | 27 |
| 3.1.2 | Conceptual uncertainty | 27 |
| 3.1.3 | Data uncertainty | 29 |
| 3.1.4 | Spatial variability | 29 |
| 3.1.5 | Temporal variability | 30 |
| 3.1.6 | Scale | 30 |
| 3.1.7 | Confidence | 31 |
| 3.1.8 | Risk | 31 |
| 3.1.9 | Error, precision, bias and accuracy | 31 |
| 3.1.10 | Deformation zones | 32 |
| 3.1.11 | Rock units and rock domains | 32 |
| 3.2 | Handling spatial variability | 33 |
| 3.3 | Scale | 34 |
| 3.4 | Handling data uncertainty | 35 |
| 3.5 | Handling alternative models | 36 |
| 3.6 | Input to scenario uncertainty | 38 |
| 3.7 | Conceptual uncertainty | 38 |
| 3.8 | Confidence | 39 |
| 4 | Concluding remarks | 41 |
| 5 | References | 43 |

1 Introduction

Development of Site Descriptive Models is an essential part of the Site Investigations carried out by the Swedish Nuclear Fuel and Waste Management Company (SKB). The site description should cover the geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties and the ecosystems of the site. The current document concerns the strategy to be used for achieving adequate integration between disciplines in this modelling and discusses some fundamental principles as regards uncertainties, alternative models and confidence assessment.

1.1 Requirements

The basic ambitions, content and principles for Site Descriptive Modelling is described in the general execution program for the site investigations /SKB, 2001/. The Site Descriptive Model should be an integrated description of the site and its regional environments with respect to current state and naturally ongoing processes, covering geology, rock mechanics, thermal properties, hydrogeology, hydrogeochemistry, transport properties and ecosystems. The description is made in Regional and Local scale and should serve the needs for Safety Assessment and Rock Engineering, /SKB, 2000/.

Even if a 'Site Descriptive Model' mainly is a description, it is still a 'model'. The selection of parameters and geometrical framework is based on an underlying conceptual model of the site. Estimation of geometry and parameter values into a full three-dimensional description rests on extrapolation of data measured at a few locations. Furthermore, the confidence in the description should be tested with simulations of e.g. groundwater flow or stress distribution to the extent useful. However, Site Descriptive Modelling does not concern simulation of e.g. the future site evolution (part of Safety Assessment) or estimation of tunnel stability (part of rock engineering analyses). The Site Descriptive Model is, of course an essential input to such simulations.

The following requirements apply for the Site Descriptive Modelling Strategy:

- 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, Investigations and Rock Engineering, 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 gathering, 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.

In addition, the modelling strategy must strive for integration. Interpretations within the different disciplines should be consistent with the interpretations made in the other discipline and should to the extent possible be used to support a unified view of the site. Furthermore, the modelling approach needs to be similar at different sites to allow fair comparison between sites.

Still, a good modelling process and good quality work must rest on the commitment and professionalism of the participants in the modelling projects. It is thus emphasised that the strategy for integrated evaluation, as described in the current document, is not a strict and detailed instruction for how to carry out such a complex task. Rather, the strategy provides some basic structure and guidance to the modelling process.

1.2 Approach to developing the strategy

The general characterisation program /SKB, 2001/ describes objectives of the site characterisation programme and provides an overview of methods for characterisation. It defines different characterisation stages and discusses the interaction needed between different disciplines. Detailed modelling and evaluation strategies have been developed for geology /Munier et al, 2003/, rock mechanics /Andersson et al, 2002a/, thermal properties /Sundberg, 2003/, hydrogeology /Rhén et al, 2003/, hydrogeochemistry /Smellie et al, 2002/ transport properties /Berglund and Selroos, 2003/ and ecosystems /Löfgren et al, 2003/. The current document addresses the integration of these efforts in a unified process.

The integrated methodology has been developed during discussions within SKB and different SKB supported modelling teams. Discussions and experiences gained during the development of the various aspects of the Site Characterisation programme have been the main source of information. In addition, the Laxemar project /Andersson et al, 2002b/ has offered an essential test bed for the modelling strategy outlined here.

1.3 This report

This report is organised as follows. Chapter 2 provides definitions of some terms, essentially related to uncertainty. Chapter 3 provides an overview of the modelling steps, with focus on the integration between different disciplines. Chapter 4 concerns assessment of uncertainty and confidence, which is an essential part of the integrated modelling work. Chapter 5 discusses documentation and Chapter 6 provides some concluding remarks.

2 Site Descriptive Modelling

The Site Descriptive Modelling is performed stepwise and entails the integration between several different scientific disciplines. This chapter provides an overview of these steps, with focus on the integration between the disciplines.

2.1 Overview

The site-descriptive model is devised and updated in a stepwise mode as illustrated in Figure 2-1.

After a completed batch of measurements, the primary data are first evaluated within each discipline; geology, rock mechanics, hydrogeology, hydrogeochemistry etc. This *evaluation of primary data* both concern quality control of data and ‘intermediate interpretations’ aiming at producing ‘building blocks’ for the three-dimensional description. This next main step, descriptive *three-dimensional modelling*, concerns estimation of geometry, properties and some basic conditions in three-dimensions. This step also includes interdisciplinary assessments of the *confidence and uncertainty* in the produced description. One way of describing these uncertainties is to produce *alternative* models. After these main steps follows *comparison* between the new and previous models, and a *discussion* on how additional measurements may affect uncertainties in prediction.

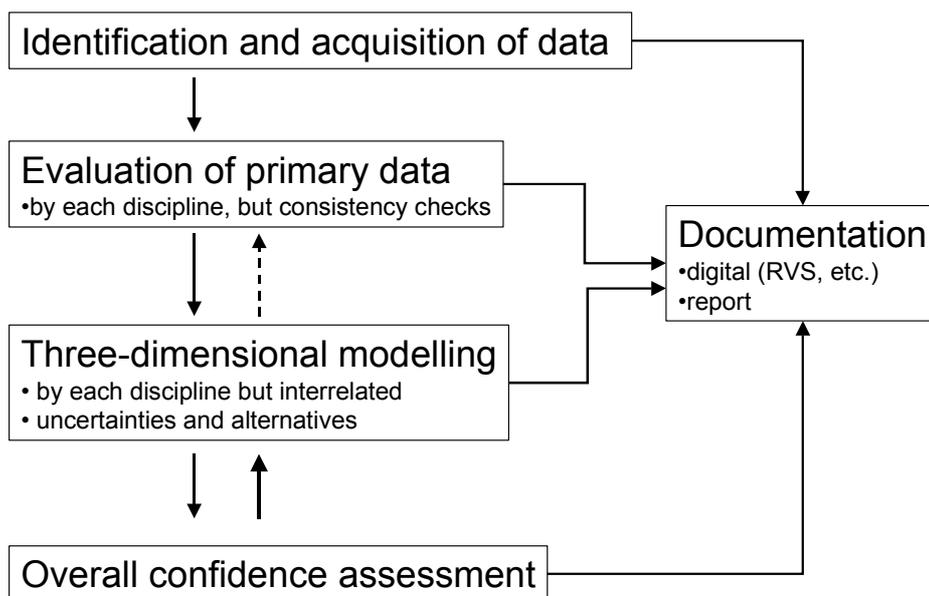


Figure 2-1. The site descriptive modelling process may be split into various components.

The updated model is delivered to the users (primarily Rock Engineering and Safety Assessment). Their assessment of the significance of uncertainties together with an assessment (essentially by the Site Modelling team) on the prospects of reducing the uncertainties, form the basis for decisions whether additional loops of modelling or data acquisition are necessary. The overall judgements lie outside the scope of the Site Descriptive Modelling.

2.2 Organisational setup

It has been found fruitful to conduct the modelling work through a project group (a ‘Site Descriptive Modelling Team’) with representatives from all disciplines. The project group should meet at regular intervals to discuss on a detailed level the current progress and ideas of the different modellers. Detailed analyses are performed within each discipline in smaller working groups targeting specific issues.

The project group meetings enable continuous cross discipline information flow and feedback; the multidisciplinary insights are hard to achieve by any other means. Yet, interdisciplinary Site Descriptive Modelling is a huge undertaking with which encompasses many sub-analyses. Attention should be paid on the following:

- The size of the working group has to be manageable and it should include the persons actually in control of the detailed analyses. A too large group will have a detrimental impact on the usefulness of the group interaction and information flow.
- If different modelling groups are used to model different sites it is essential that the work is sufficiently co-ordinated allowing for later inter-comparison between the sites. There has to be co-ordination in judgements, presentational styles etc.
- The evaluation is a learning process – and takes time. There is a need to get acquainted with the site and its data but also the nomenclature and modus operandi of the various sub-groups.
- Three-dimensional interpretation and visualisation techniques are essential both for the geometric modelling and for communication of results within the group.
- Flexible, easily accessible and yet quality assured procedures for project information management are essential.

Finally, a substantial amount of documentation is produced when aiming for traceability. Careful documentation also takes time. While extensive documentation is essential for the end products produced during the Site Investigation (e.g. after completion of the Initial Site Investigation and after completion of the Complete Site Investigation), less ambitious documentation may be contemplated for the intermediate versions of the models.

2.3 Evaluation of primary data

The primary (i.e. the ‘measured’) data constitute a wide range of different measurement results. These data both need to be checked for consistency and to be interpreted into a format more amenable for three-dimensional modelling.

2.3.1 Assembling primary data

The Site Descriptive Models should rest on fully traceable records of its information sources. Furthermore, the ambition level should be that each model version should consider all relevant data, as this will enhance confidence in the model (see section 3.8). The only reason not to consider data is if the quality of the data is questionable.

At a given iteration there will be three main sources of information:

- previously acquired primary data used in previous model versions,
- interpretation of the previous data into previous model versions and
- data not previously considered in earlier model version (i.e. normally the new data).

The investigation results (primary data) are mainly stored in the SKB databases SICADA and the SKB SDE (GIS) databases. Most of the SICADA data are measurement results or results from evaluations of such data, stored in tables. Apart from direct measurement results, these databases may also contain evaluated data such as ‘single borehole interpretations’. Data should be retrieved using the purpose-designed software and procedures. The export format varies according to the importing software, e.g. RVS and WellCad have specific import routines connected to the SICADA structure.

There may be a need to consider data not stored in the in the official and Quality Assured databases. This may, for example concern experiences from construction works in the vicinity or other assemblies of historical records. If such data are used, special and documented efforts are needed for assessing the quality of the information.

Previous model versions (if they exist) are stored in RVS and in written documents. In the next iteration, teams are, with some restrictions, free to change interpretation – but all changes need to be documented and justified (see section 2.5).

A set of documents (appendices to the modelling report) should be compiled, which should make it possible to trace the information from SICADA and RVS and how the data were used for producing the model. Specific instructions (protocols) could be developed in the modelling projects, see e.g. chapter 5 in /Andersson et al, 2002a/.

2.3.2 Evaluating primary data within each discipline

While cross-discipline interpretation is encouraged, there is also a need for transparency. This means that the evaluations are first made within each discipline and thereafter compared in a cross-discipline manner to check for potential inconsistencies. However, the other disciplines should be kept fully informed, e.g. through the project group meetings, on the progress of these evaluations.

The different investigation teams, i.e. the site organisations, may already have done some of the evaluation of the primary data. The Site Descriptive Modelling Teams need then only check that this evaluation has been conducted according to instructions and in a comparable manner. Furthermore, data used and evaluated in previous model versions would primarily not need to be re-evaluated and could, after a quality check, be re-used directly in the three-dimensional modelling. However, the Site Descriptive Modelling Teams have the right to re-evaluate previously analysed data whenever warranted. A reason for this could be to search for evidences of features not considered in previous versions or to test new insights on how to assess the primary information.

Geology

/Munier et al, 2003/ summarise the geological evaluation of the primary data. The generic geological knowledge as well as findings from some of the surface based investigations are combined into a description of the geological historical evolution, using 'standard methods' of the geological science. Arguments based on this geological evolution are often essential for justifying extrapolation of shape and size of units and of arguing size and direction of fracture zones. The surface information is also used for compiling surface geology (rock type) maps and lineament maps. Borehole geophysics and geological borehole logs are interpreted into a unified geological description along each borehole. This geological single-hole interpretation also identifies potential fracture zone intersections with the borehole. The measured signals from reflection seismics and borehole radar can be interpreted into reflectors or reflection cones. These reflectors are then used in the three-dimensional modelling. Lineaments and fracture data are evaluated statistically into a fracture statistical description.

Hydrogeology

/Rhén et al, 2003/ summarise the hydrogeological evaluation of primary data. The surface hydrology data are compiled into a surface hydrogeological description. The pressure and water level monitoring data are assembled. The different hydraulic tests carried out in the boreholes are interpreted into a hydrogeological single-hole interpretation of the permeability distribution along the boreholes and identification of potential hydraulic conductor intersections and some correlation studies of mapped core versus permeability distribution.

Hydrogeochemistry

For hydrogeochemistry the primary data evaluation essentially concern quality checks of the collected water samples /Smellie et al, 2002/. The evaluation essentially aims at identifying representative data sets for the further analysis.

Rock Mechanics

According to the rock mechanics modelling strategy /Andersson et al, 2002a/ the primary data evaluation concerns assessment of stress measurements, assessment of mechanical tests and bore cores etc, rock mechanical interpretation of borehole data and a joint rock mechanics and geological evaluation of borehole data.

Thermal properties

/Sundberg, 2003/ lists the various sources of information for temperature and thermal properties. Direct measurement includes in-situ temperature measurements and thermal tests on bore cores. However, the three dimensional description requires establishment of good correlation between aspects of the geological description, like mineralogy or density, and the thermal properties.

Transport properties

/Berglund and Selroos, 2003/ describe the procedures for obtaining parameters for radionuclide transport modelling. Several of these parameters are flow-related transport parameters and are mainly obtained from flow modelling. However, there is a need to do a primary evaluation of data resulting from the laboratory programme intended to obtain primarily retention properties of the rock matrix. Furthermore, some in-situ techniques may be employed to obtain transport parameters; in this case a primary evaluation of data is also needed.

Ecosystems

/Löfgren et al, 2003/ develop the strategy for development of an ecosystem site descriptive model.

2.3.3 Interdisciplinary comparisons

After a first attempt of the discipline specific evaluation of the primary data should follow a phase of interdisciplinary comparisons. Generally, these comparisons should check for potential consistency or inconsistency between disciplines and also to check if specific observations find support in more than one discipline. Such comparisons would be particularly valuable for the geological and hydrogeological single hole interpretations. Is there hydraulic support for the potential fracture zones and vice versa? The results of the intercomparisons should be added to the interpretation, but not revise them – unless obvious mistakes are found.

2.4 Descriptive modelling in 3D

The three-dimensional modelling essentially concern estimation of geometry and properties in three-dimensions. SKB has presented a methodology to construct, visualise and present the Site Descriptive Models /Munier and Hermanson, 2001/. The main tool for interpreting and visualising geometrical information in three dimensions is the Rock Visualisation System (RVS) – a Microstation-based 3D visualisation and modelling software package developed by SKB, but the modelling and its documentation is not restricted to this tool.

Of special consideration is the fact that there usually exist previous model versions. The information in the past versions needs to be considered. In the next iteration, teams are, with some restrictions, free to change interpretation – but all changes need to be documented and justified.

2.4.1 Selecting the model domain

According to plan /SKB, 2001/ a Regional and a Local descriptive model should be developed (updated) in each iterative step. After reviewing the available information an early step in the modelling will be to determine the size and location of these model domains. For the RVS representation a defined volume is needed. As discussed and explained by /Munier and Hermanson, 2001/ the predictions should cover the entire volume of a model domain and be of the same resolution (scale), although the confidence may vary in different parts of the model domain. This does not mean that the verbal descriptions of the site need to be restricted to the size of the RVS-representation. Also, boundaries of numerical models used in subsequent analyses need not coincide with the RVS-representation boundary. Selection of boundaries and boundary conditions is left at the discretion of the modeller and should be decided on the purpose of the modelling, but it is of course an advantage if the boundaries do not extend beyond the boundaries of the RVS representations.

In addition, the following may be considered for making the selection of the model domain:

- The Local Site Descriptive Model should cover an area of about 5–10 km², i.e. large enough to include the potential repository and its immediate surroundings. This also means that the location of the model area needs to be agreed between Rock Engineering and the Site Modelling groups. The Regional Descriptive Model should be large enough to provide boundaries and site understanding to the Local Model.
- If possible, model domains selected in previous versions should be retained. Deviations should be carefully motivated.
- The models should include the main sources of information (e.g. the deep boreholes and areas of intensive surface geophysics).
- The Local domain should be large enough to allow meaningful hydrogeological flow simulations, even if information for boundary conditions or an encompassing regional scale hydrogeologic model may need to be taken from the Regional domain – or beyond.
- Potentially important features, lineaments rock type boundaries etc should be considered when selecting the size.
- For practicality, the model domains should not be too large in relation to the selected resolution (scale) of the description.

2.4.2 Estimating structures and properties in three dimensions

Three-dimensional modelling, i.e. estimating the distribution of parameter values in space, is made in a sequence where the geometrical framework is taken from the geological model sustained by multidisciplinary (i.e. not only geological) evaluations of the primary data. The geometrical framework is in turn used by rock mechanics, thermal and hydrogeological modelling. The thermal model is essentially based on the lithological description of the geological model. The hydrogeochemical description is to some extent developed independently, but its consistency with the hydrogeological description must be ensured. The description of transport properties is based on the

hydrogeological and hydrogeochemical descriptions, although additional data are assessed as well. Finally, the description of the near surface is made essentially independent of the other descriptions, but the interface between geosphere and biosphere is handled jointly with, essentially, hydrogeology. Even if most of these first steps in the development chain are made within each discipline, the other disciplines must be kept adequately informed, e.g. through the project group meetings, on the progress of these evaluations.

The first question to be asked within each discipline is to what extent previous model versions would suffice to explain the new, evaluated data. The outcome of this comparison, which should be documented, would then guide the approach for developing the new model versions.

If found reasonable, one way of generating a new version could be to just update the old version, by e.g. reviewing and adjusting each geometrical structure, search for evidences of additional structures and by updating the property estimates inside rock domains etc. However, the question should always be asked if totally new model (with alternatives) needs to be developed. Uncertainties are estimated, see chapter 3.

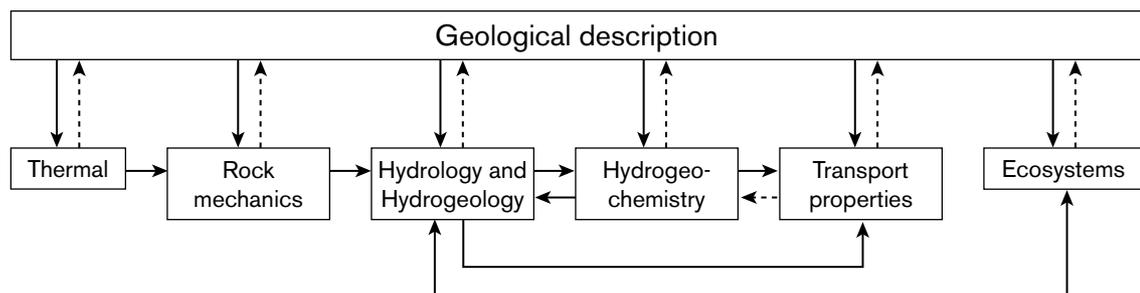


Figure 2-2. The different discipline descriptions are interrelated with several feedback loops and where geology provides the essential geometrical framework.

Geology

The Geological Site Descriptive Model only explicitly (deterministically) describes the fracture zones with a size larger than around 1 km. Such zones are called ‘regional zones’ (>10 km) and ‘local major zones’ (1–10 km). The remaining zones are described statistically within each rock domain. Identification of zones is mainly made from the lineament maps, the single-hole interpretation of the boreholes and from seismic and radar reflectors, see Figure 2-3 and /Munier et al, 2003/.

The geometrical distribution of rock properties and fracturing is described /Munier et al, 2003/ using the concepts of *rock units* and *rock domains* (see section 3.1.11). The interpretation is mainly based on the surface geological description, combined with the single-hole interpretations of the boreholes.

The geological description thus includes both a geometrical framework (deformation zones and rock domains) and parameter values describing these domains. The spatial variability and uncertainty of the parameter description should be described (see sections 3.2 and 3.4). In addition, there is usually reason to develop alternative geometrical frameworks (see section 3.5) to handle uncertainties in the overall geometry. In this first step of development, the uncertainty evaluation should be based on the geological information, later steps will add information from other sources.

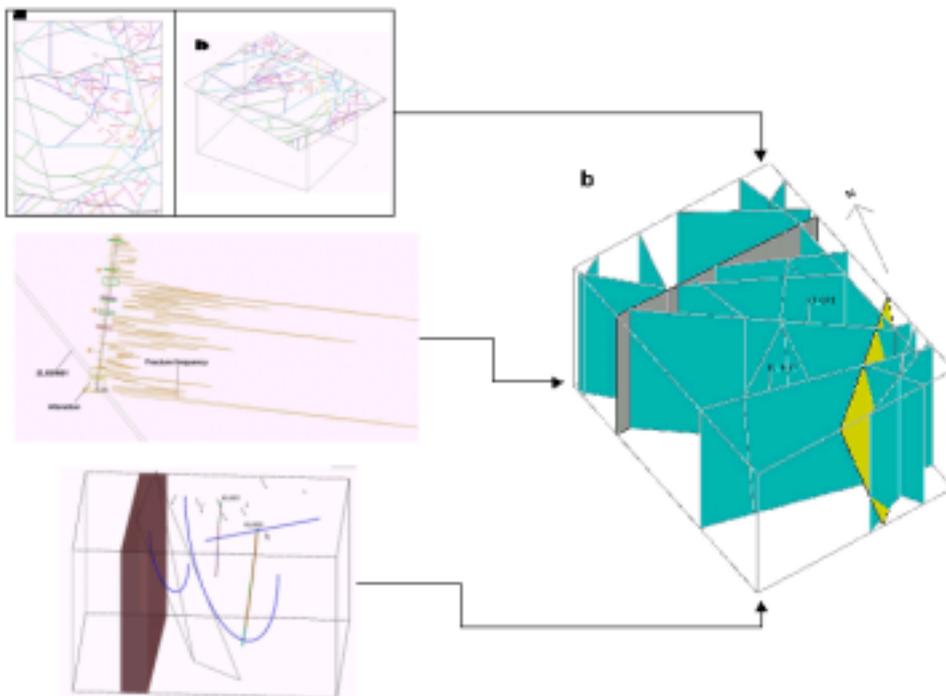


Figure 2-3. Identification of deformation zones in 3D is mainly made from the lineament maps, the single-hole interpretation of the boreholes and from seismic and radar reflectors (example developed from /Andersson et al, 2002b/).

Rock mechanics

SKB has developed a Rock Mechanics Site Descriptive Modelling Strategy /Andersson et al, 2002a/. The model describes the initial stresses and the distribution of deformation and strength properties of the intact rock, of fractures and fracture zones, and of the rock mass. The spatial variability and uncertainty of the parameter description should be described (see sections 3.2 and 3.4). Rock mass mechanical properties are estimated by empirical relations and by numerical simulations but overall judgement is finally needed. The stress modelling approach integrates stress measurement data, geological factors, numerical modelling and the uncertainties involved. The geological description is a very important input both to the determination of rock mechanics properties and to the stress modelling.

The rock mechanics modelling team should assess the uncertainties in their description. After this, the reasonableness of the geological description in relation to the rock mechanics data should be assessed and later discussed in the joint evaluation, see section 2.5.

Thermal properties

The three-dimensional description of the thermal properties needs to rest on correlation between aspects of the geological description, like mineralogy or density, and the thermal properties. The thermal property modelling team should also assess the uncertainties in their description. /Sundberg, 2003/ discusses how the modelling should be accomplished in practice.

Hydrogeology

The hydrogeological description /see Rhén et al, 2003/ primarily concerns information on the permeability distribution at various scales (resolution) for the deterministic deformation zones and the rock domains. The spatial variability and uncertainty of the parameter description is described, using both continuous and discrete representations (see sections 3.2 and 3.4). The geometrical framework is based on the geological description of the rock domains and associated rock units (see Figure 2-4), but the hydrogeological evaluation of data may lead to further divisions into different units, or to combining geologically distinct units into hydraulic domains with the same (statistically) hydraulic properties. The hydraulic description may in turn be used for (numerical) simulation of different tests (e.g. interference tests) and measurements (i.e. salinity distribution) for further calibration or assessment of confidence in the model.

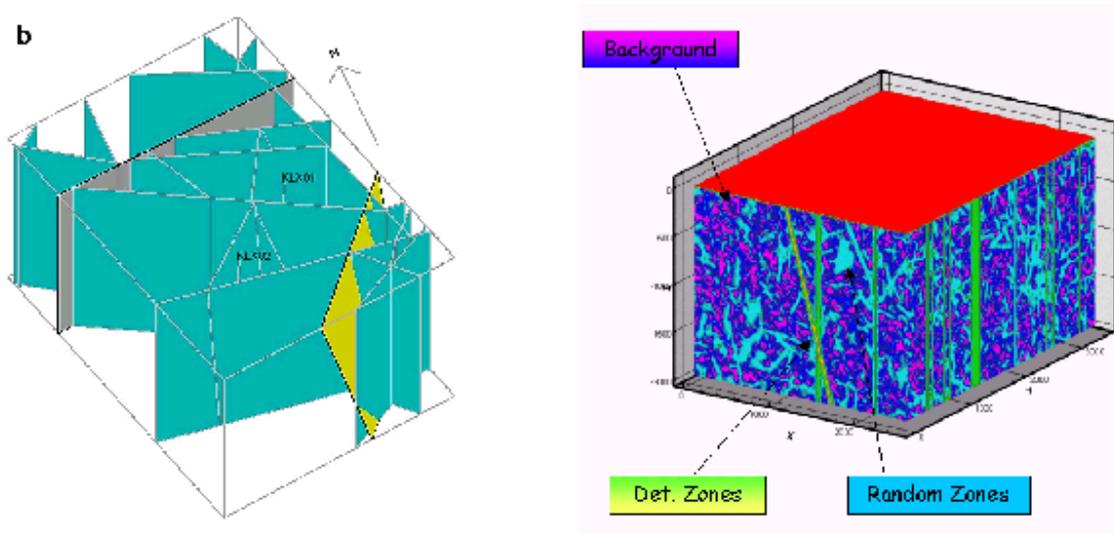


Figure 2-4. The geometrical framework in the hydrogeological description is based on the geological description of the rock domains and deformation zones, but the higher resolution description is made stochastically (developed from figures in /Andersson et al, 2002b/).

The hydrogeology modelling team should assess the uncertainties in their description. After this the reasonableness of the geological description in relation to the hydrogeology data should be assessed. For example, the question may be asked whether the current geometrical structures allow a reasonable interpretation of interference tests. The findings should later be discussed in the joint evaluation, see section 2.5.

Hydrogeochemistry

/SKB, 2001/ has defined the major task for hydrogeochemical evaluation to include:

- Characterise undisturbed groundwater chemistry including the origin, depth/lateral distribution and the turnover time.
- Focus on data of importance for the safety evaluation such as pH, Eh, chloride, sulphide, colloids and microbes.
- Identify possible dissolved oxygen at repository depth.

/Smellie et al, 2002/ have developed documented procedures for the hydrogeochemical modelling to be used to attain these goals. The data evaluation becomes a complex and time-consuming process when the information has to be decoded. Manual evaluation, expert judgement and mathematical modelling is often combined dependent on the aspect of the modelling. The predicted water distribution can also be compared with simulations made on the hydrogeological description.

The hydrogeochemistry modelling team should assess the uncertainties in their description. After this the reasonableness of the geological and the hydrogeological descriptions in relation to the hydrogeochemistry data should be assessed and later discussed in the joint evaluation, see section 2.5.

Transport properties

/Berglund and Selroos, 2003/ present the methodology for constructing the 3D transport description. In short, retention parameters are assigned to different geological units in accordance with the geological description. Flow modelling identifies transport paths through the modelling domain for relevant flow conditions. Finally, effective transport parameters for use in subsequent transport modelling are obtained through proper integration of flow and retention characteristics along the transport paths.

The transport modelling team should assess the uncertainties in their description. After this the reasonableness of the geological, hydrogeological and hydrogeochemical descriptions in relation to the transport data should be assessed and later discussed in the joint evaluation, see section 2.5.

Ecosystems

The site-specific investigations will result in site descriptions that will characterise and quantify patterns and processes important for the ecosystem in a broad sense. These descriptions will constitute the basis for future modelling, such as the safety analysis, and the EIA, although additional information will be included for the later purpose. The safety analyses will use an ecosystem approach were possible paths of transport and accumulation of radionuclides will be analysed by modelling biogeochemical circulation processes.

The surface ecosystem modelling team should assess the uncertainties in the description. After this the reasonableness of the geological, hydrogeological and hydrogeochemical descriptions of the geosphere/biosphere interface in relation to the near surface data should be assessed and later discussed in the joint evaluation, see section 2.5.

2.5 Overall evaluation of confidence

After the individual discipline modelling and uncertainty assessment a phase of joint overall confidence evaluation follows. Relevant parts of the different modelling teams assess the suggested uncertainties and assess the feedback, in particular to the suggested geology, hydrogeology and hydrogeochemistry descriptions. Based on this assessment, the modelling teams may need to update their descriptions.

After these revisions the teams re-assess the model description with its uncertainty and confidence statements. These discussions should assess overall confidence by:

- checking that all relevant data are used,
- checking that information in past model versions is considered,
- checking consistency (i.e. no conflicts) between the different discipline model interpretations, like possibility to predict measured salinity distribution, see Figure 2-5,
- checking that the different kinds of uncertainty listed in chapter 3 are addressed,

- checking if suggested alternatives make sense and if there is potential for additional alternatives,
- and by discussing, if appropriate, how additional measurements (i.e. more data) would affect confidence.

The findings as well as the modelling results are to be documented, see chapter 2.6.

As regards the suggestions for additional measurements, it is essential that for each suggested additional measurement its potential benefits in terms of how it could affect uncertainty and confidence is addressed. More specifically, at some point during the site investigation there will be a diminishing return on the value of additional data. Furthermore, it is primarily the end users (rock engineering and safety assessment) who could assess to what extent the uncertainty and confidence impact their analysis. The final decision whether additional measurements are indeed needed or worthwhile can only be made by the SKB management (e.g. by the “central site evaluation” group). Still, the confidence assessment and the evaluation of the potential use of additional data would be essential input to this decision process.

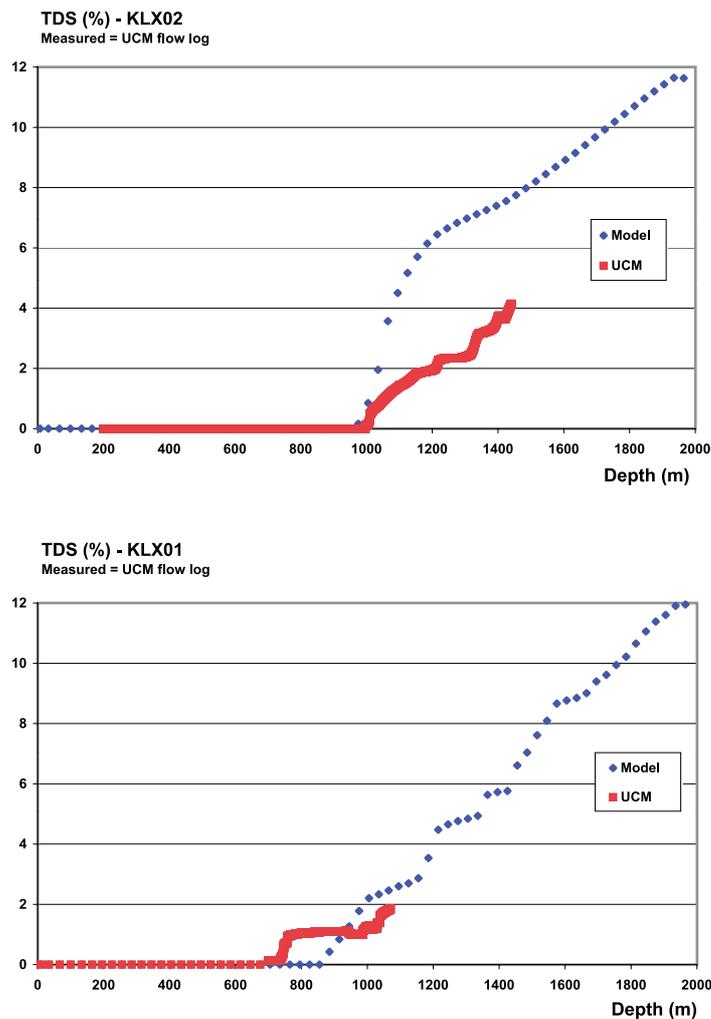


Figure 2-5. Successful comparisons between the hydrogeological prediction of salinity levels and actually measured levels enhance confidence /from Follin and Svensson, 2002/.

2.6 Documentation

The Site Descriptive Modelling results in a Site Description /see SKB, 2001/. This description encompasses the different databases and digital models developed as well as a model report with associated sub-documentation. This chapter provides an overview of the documentation needs.

2.6.1 Digital information

The digital model information is stored using the Quality Assured SKB databases and mainly using the RVS-system, as discussed by /Munier and Hermanson, 2001/. More detailed instructions are provided in the different discipline specific modelling strategy reports. In case digital information is produced, which cannot be readily stored in the SKB databases, careful documentation of the character and other properties of these data need to be supplied.

2.6.2 The model report

Main model versions should be documented in a model report. These model reports are certainly required after the completion of the Initial Site Investigation and after the completion of the Complete Site Investigation, but intermediate reports may also be produced. The outline of the Methodology Test for Site Descriptive Modelling /Andersson et al, 2002b/ may be used as an inspiration, but need of course not be followed literally.

Nevertheless, it is essential that the report should cover the following:

- References to **data sources** and identification of **previous model versions**.
- Means of **primary data evaluation** including; the disciplinary evaluation, re-evaluation of previously evaluated data and means of interdisciplinary comparisons.
- Means of **three dimensional modelling** including the disciplinary evaluation with its comparisons with previous model versions, uncertainty estimates and the joint uncertainty and confidence evaluation.
- Presentation of the **Site Descriptive Model** (discipline by discipline) with its uncertainties and alternatives as well as the overall confidence in the description (i.e. the result of the overall evaluation).
- **Comparison** with previous model versions, assessment on **overall confidence** and discussing potentially fruitful additions to the **measurement programme**.

Model reports for different sites should follow the same outline. A standardised outline is preferable and should be developed in time for the Site Descriptive Model reports produced after the Initial Site Investigation. Still, modifications of this outline may be needed during the Complete Site Investigation.

3 Assessment of uncertainty and confidence

There are always uncertainties in interpreting measurements and rock parameters, which vary in space. The three-dimensional description should present the parameters with their spatial variability over a relevant scale, with the uncertainty included in this description. Different alternative descriptions may be required. In addition, it is also necessary to describe the confidence in the model predictions.

3.1 Definitions

In order to avoid misunderstanding it is important to use a common nomenclature within the Site Descriptive Modelling. In particular, there is a need for a common nomenclature regarding uncertainty, as there are different kinds of uncertainty and its origins vary. Definitions are provided below, which are based on international practise but adapted to the way these terms are used within SKB. These definitions should, if at all possible, be used by all involved in the modelling and in the interface with other activities.

3.1.1 Scenario uncertainty

Scenarios and scenario uncertainty is generally the uncertainty in the future site and repository evolution, which depend on uncertain future external events or boundary conditions. Examples of such changes are climatic change, future human actions or very large-scale tectonic events.

Scenario analysis is an essential component of a Safety Assessment and is not made for the Site Description (see also 3.6). The evolution of external events is a continuous development, which cannot be predicted in its full detail. In order to get a handle on this development, a number of future events or conditions, which can initiate chain of events – scenarios – are selected. Analysing the selected scenarios provides a handle on the range of possible, future evolution. The selection of scenario initiating events and conditions are made by expert judgement, see e.g. SR 97 /SKB, 1999a/.

3.1.2 Conceptual uncertainty

Conceptual uncertainty concerns the uncertainty originating from an incomplete understanding of the structure of the analysed systems and its constituent interacting processes. The uncertainty is comprised both of lack of understanding of individual processes and the extent and nature of the interactions between the processes (Figure 3-1).

For the Site Descriptive Model, incomplete understanding of the basic geometrical structures of the rock is also a conceptual uncertainty (Figure 3-2). Within geology it is also quite common to denote uncertainties in the properties of the geometrical model – such as the number and position of fracture zones – as conceptual uncertainties, but these uncertainties are related to data uncertainties (see below). The use of ‘conceptual uncertainty’ in this context is not supported here and should be avoided in the Site Descriptive Modelling.

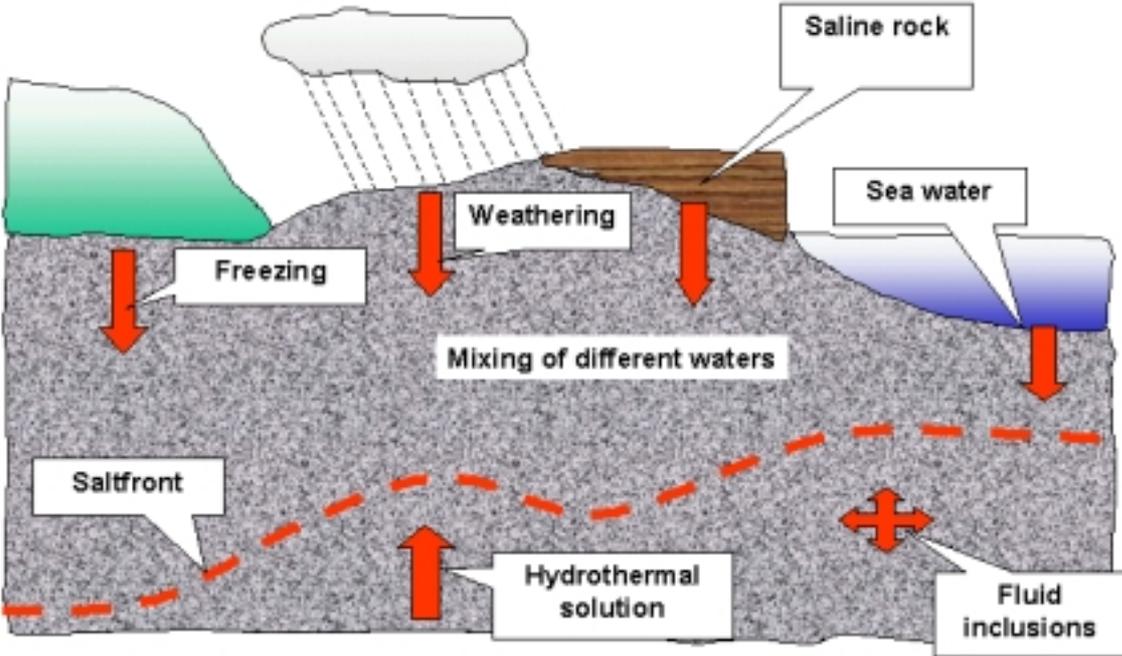


Figure 3-1. A conceptual model of groundwater processes determining groundwater composition – but all these processes may not be important (illustration developed from Laaksoharju, pers. comm.).

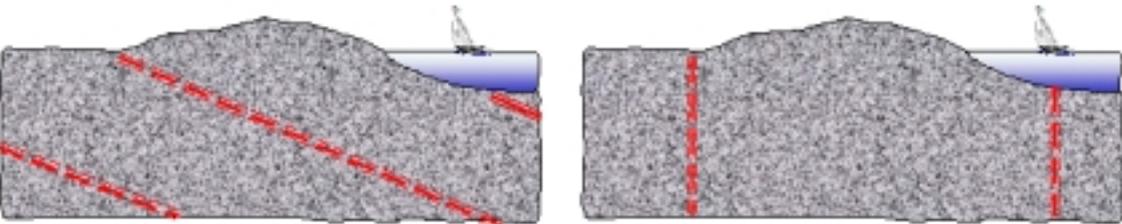


Figure 3-2. Prior to investigations aiming at the subsurface there may be a conceptual uncertainty whether deformation zones tend to be subhorizontal or more subvertical. This conceptual uncertainty will be resolved during a Site Characterisation. Note, that the precise dip of deformation zone may still be uncertain, but this is data uncertainty – not conceptual uncertainty.

3.1.3 Data uncertainty

Data uncertainty concerns uncertainty in the values of the parameters of a model, i.e. uncertainty regarding the properties. Such uncertainties may be caused by, for example, measurement errors, interpretation errors, or the uncertainty associated to extrapolation of parameters that varies in space, and possibly also in time. Conceptual uncertainty can cause data uncertainty, see e.g. Figure 3-3.

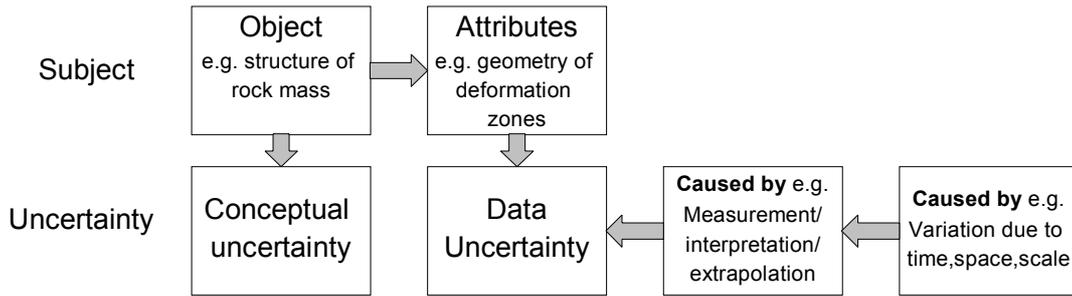


Figure 3-3. Conceptual uncertainty, data uncertainty and spatial variability may all be related.

3.1.4 Spatial variability

Spatial variability concerns the variation in space of a parameter value. Spatial variability is very common in the bedrock. Hydraulic properties along a borehole usually display significant spatial variability as seen in Figure 3-4. The variability is not uncertain (it is a property of the rock), but implies uncertainty estimated hydraulic properties further away from the borehole.

Spatial variability is not uncertainty *per se*, because it can be well recognised and understood, but it is often a cause for data uncertainty. Parameters with strong spatial variation are difficult to evaluate beyond the local region of their measurement.

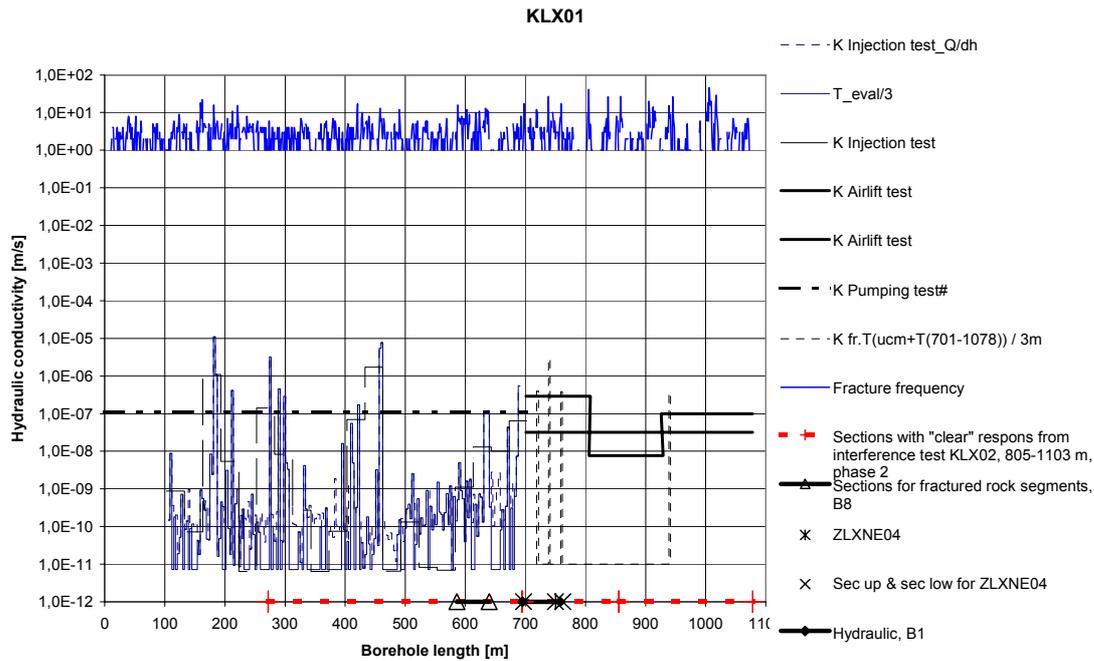


Figure 3-4. Hydraulic properties along a borehole usually display significant spatial variability. The degree of variability is also a function of scale (see section 3.1.6 below). The variability is not uncertain (it is a property of the rock), but implies uncertainty in estimated hydraulic properties further away from the borehole /from Andersson et al, 2002b/.

3.1.5 Temporal variability

Spatial variability concerns the variation in time of a parameter value. As with spatial variability, temporal variability is not uncertainty per se, because it can be well recognised and understood, but it is often a cause for data uncertainty. It should be noted that most basic geologic conditions at a site show very little temporal variability over the time of interest for repository performance, but e.g. hydrogeologic boundary conditions – not to mention conditions and properties at the surface – vary in time.

3.1.6 Scale

Scale concerns the spatial resolution of the description. For a spatially varying property, the scale is the size of the domain over which properties are averaged. Spatially varying properties will manifest different values when described at different scales (see Figure 3-4). For example, using a high resolution description, i.e. at the ‘small scale’, intact rock and fractures would be described as individual entities but, at the larger scale, the descriptions would be combined into a ‘rock mass’ value. Scale should *not* be confused with accuracy or precision (see below).

The scale also affects the values of properties defined as (volume) averages such as rock mass mechanics properties or hydraulic conductivity – which are scale dependent. In a high-resolution description, fracture zones and large fractures will be given their own mechanical and hydraulic properties and will thus not be included in the averages representing the rock mass in-between these features. In a description with less resolution these features (with significant impact on the properties) will be included in the averages.

3.1.7 Confidence

The confidence in a descriptive model is the total assembly of motives, indications, and arguments in support of the model. However, high confidence is not synonymous to low uncertainty. If the uncertainty description is well founded, the confidence can be high in the model. Conversely, if a model description with low uncertainty has a poor foundation, the confidence in the model should be low. Sometimes the word ‘validity’ instead of confidence, but this word is not advocated here.

3.1.8 Risk

Risk is a joint assessment of probability and consequence. Often, but not always, risk is calculated by multiplying the probability of an event by its consequence. The overall risk is obtained by adding the risk contribution of individual independent events into a total risk estimate. Risk criteria are provided in the regulations /e.g. SSI, 1998/.

Risk evaluation is an essential component of a Safety Assessment, but should not and could not be made for the Site Descriptive Models. Rather, Site Descriptive Models provide a support for risk evaluation by the parameterisation and uncertainty estimation of the site properties.

3.1.9 Error, precision, bias and accuracy

Error is the deviation between an estimate and the true value. *Accuracy* is the degree to which the mean of repeated measurements deviates from the true value, the difference being the *bias*. *Precision* is the spread of repeated values. Thus, measurements can be accurate, even though they are not precise. Figure 3-5 outlines these concepts.

Errors in the predictions or measurements, based e.g. on reading values from measurement instruments or calculating values from numerical models, may have different characteristics that should be properly described in order to properly handle the resulting uncertainty.

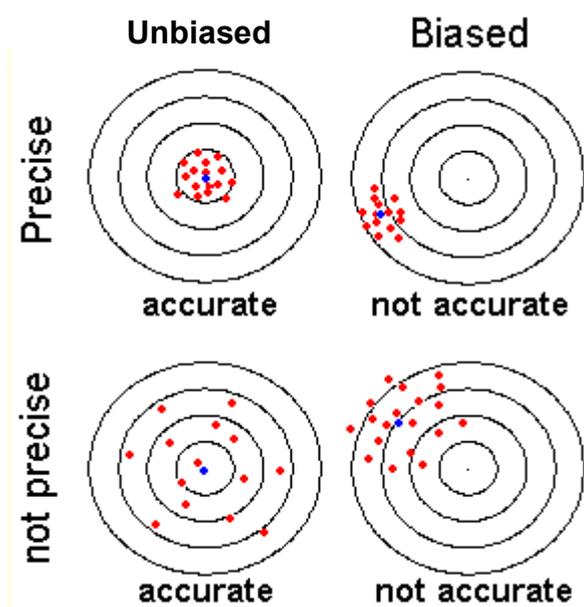


Figure 3-5. Accuracy, precision and bias.

3.1.10 Deformation zones

The term deformation zone denotes essentially two dimensional geological structures in which plastic and/or brittle deformation can be positively demonstrated. *Fracture zones* and *ductile shear zones* represent subgroups of deformation zones and are characterised by predominant ductile- and brittle deformation respectively.

3.1.11 Rock units and rock domains

A *rock unit* is a volume of rock judged to have a reasonably statistically homogeneous distribution of e.g. lithology and fracturing. A rock unit may contain several different rock types judged to be similar. A rock unit may also contain small scale inclusions of very different rock types. Each rock unit is defined by its location and is described in terms of rock type distribution and fracture- and fracture zone statistics.

Several rock units, e.g. those just separated by different fractures zones, may have similar properties. This information is also handled by logical connections in the geological model, where several rock units are assembled into *rock domains*. A rock domain is a region of the rock for which the properties can be considered essentially similar in a statistical sense, see also /Munier et al, 2003/.

3.2 Handling spatial variability

It is necessary to describe the spatial variability of the rock properties. Of specific importance is the auto-correlation, i.e. to what extent a property value at a certain point is correlated to the property value at another point in space. There are different models available for describing spatial variability and the auto-correlation structure:

- In simple cases, a stochastic variable with a certain distribution function, or a constant value, is attributed to each rock domain. This representation is used for e.g. the rock type distribution in the geological model or the rock mass properties in the rock mechanics model. Some parameters, like rock stress, may also vary in a simple manner (like a linear trend) within the rock domain.
- In other cases more sophisticated description of the auto correlation in space is needed. For continuous parameters correlation could be described using a correlation function or variograms, which is the representation used as one of the representation in the hydrogeological model (Figure 3-6). Different rock domains may take different functions.
- Volumes and surfaces (e.g. fractures) are often better viewed as stochastic objects in space. This is the basis for discrete stochastic representations, such as discrete fracture networks (see Figure 3-7) in the fracture description in the geological model and in the (alternative) discrete representation of the hydrogeological model. Different rock domains may be associated with different descriptions.

Evidently the model for describing spatial variation needs to be defined and the method used to estimate its parameter and the uncertainty in the parameters need to be described, see section 3.4. Different simulations tools usually have defined models for handling the spatial variability.

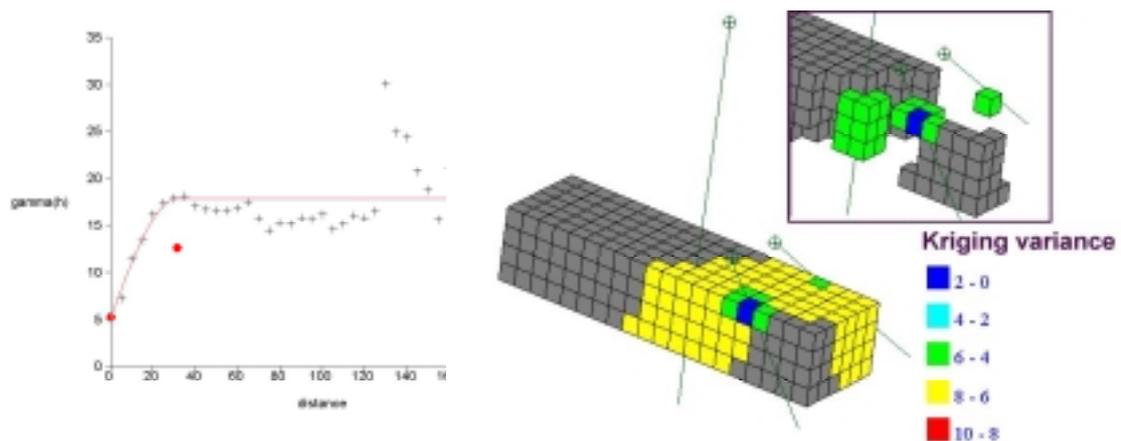


Figure 3-6. For continuous parameters correlation could be described using variograms. Close to measurement points the uncertainty (illustrated as kriging variance in the figure) is lower than further away /from Andersson et al, 2002a/.

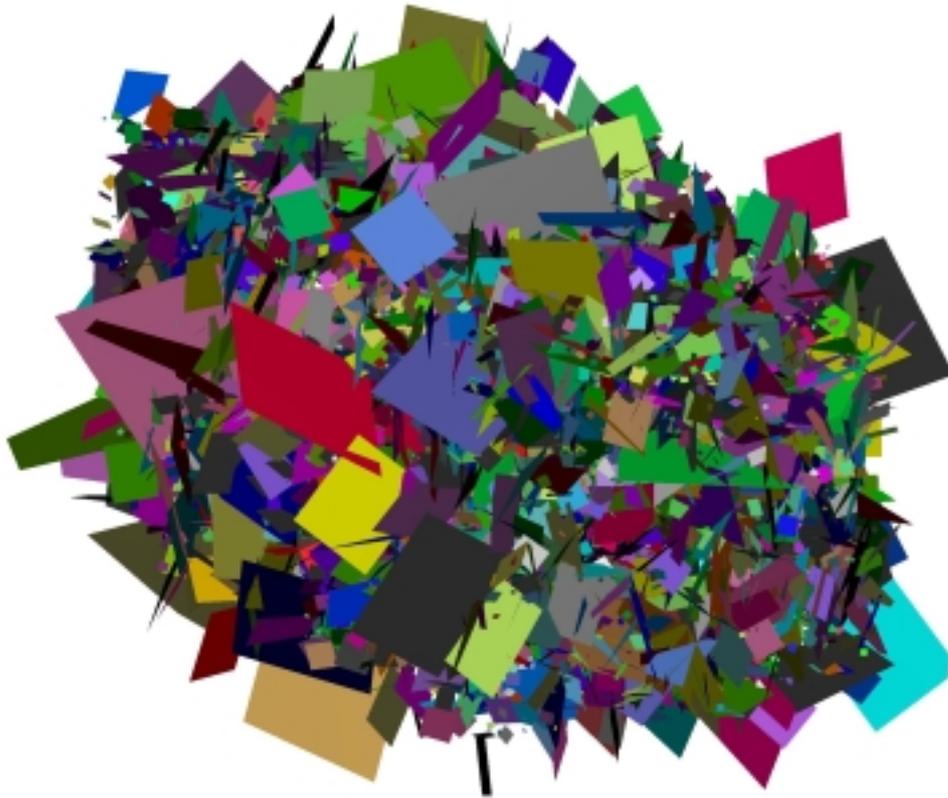


Figure 3-7. An example of a discrete fracture network representation (Stigsson pers. comm.).

3.3 Scale

The parameter values provided in the Site Descriptive Model should be associated with the scale of the description. The used scale should be adapted to the resolution needed by the users, i.e. mechanical properties should be described in ‘tunnel scale’ (30 m), see /Andersson et al, 2002a/.

The selected scale affects the spatial variability and the uncertainty in the description, see Figure 3-8. Averaging over a large scale implies that the spatial variation decreases at this level of resolution. Thus, the scale needs to be given for any estimate provided.

The user – not the modeller – should decide on the scale, as it is connected to the needs of subsequent analysis. If the modeller judges there is too little information for accurate estimates at a given scale, the modeller should handle this by increasing uncertainty (or decreasing confidence) and not by reducing the resolution in the description.

It should also be noted that different users may have different needs of resolution, which may require descriptions in different scales. For example, design issues concern tunnel scale (e.g. around 30 m), which implies a need for both mechanical and hydrogeological descriptions at this scale, but radionuclide transport modelling also requires a hydrogeological description at higher resolution (at canister scale around 5 m).

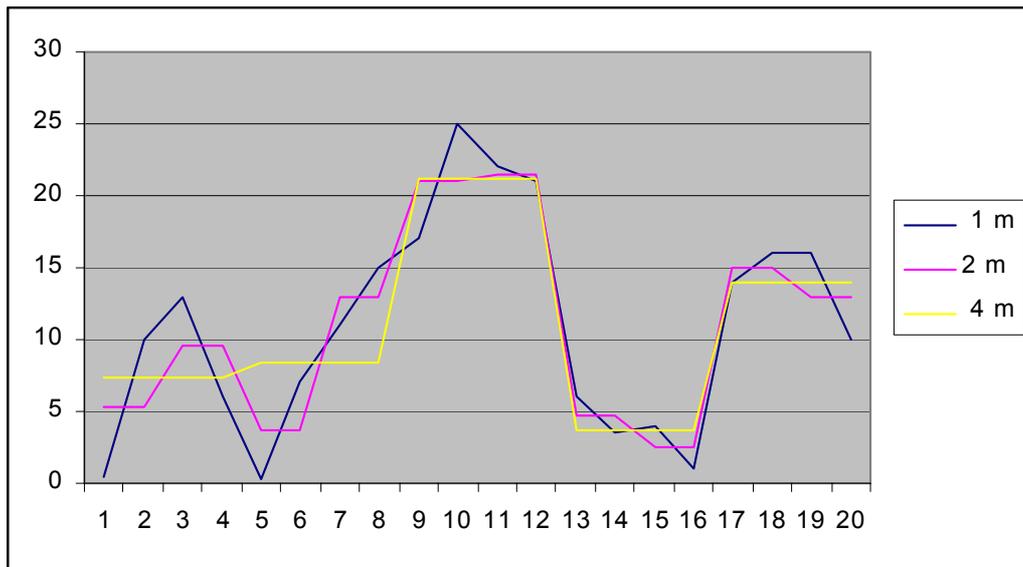


Figure 3-8. Description of a parameter in different scales (as averaged over 1, 2 or 4 m). The decreasing resolution tends to smooth the variability.

3.4 Handling data uncertainty

The Site Descriptive Model shall quantify the data uncertainty in its parameter values. This description concerns uncertainty in the parameters describing spatial variability due to a limited number of sampling points, but also other sources of uncertainty. The latter could for example be measurement errors or interpretation uncertainties of the primary information (e.g. interpretation of hydraulic tests, stress measurements etc).

Data uncertainty can be represented by different means, including stochastic variables (for single parameters) and stochastic processes (for uncertainty in functions). The representation could be discrete or continuous. The sophistication of the description depends on the character of the uncertainty but also on the importance of the parameter. Sometimes a single representative value is sufficient, but at other instances users may require a detailed description of the uncertainty.

Uncertainty estimates may be obtained using standard statistical estimation techniques, but attention is needed when there are few, unreliable or partially biased data. The statistical spread in the measurements may be a poor representation of the actual uncertainty and additional judgements of the confidence may be needed.

Data uncertainty need not only be quantified, its origin should also be described. The origin of the uncertainty is crucial in understanding how and if the uncertainty may be reduced if need be.

The data uncertainty in the Site Descriptive Model is the source of information for uncertainty analyses in Safety Assessment and in Rock Engineering Analyses. However, the actual numbers and distributions used are selected based on the purpose of these analyses – they cannot be specified in the Site Descriptive Model. For example, it is not possible to identify “pessimistic values” in the Site Descriptive Model,

this can only be done in a Safety Assessment context where the word “pessimistic” can be related to the consequences analysed. In SR 97 the selection of data and the quantification of uncertainties for the Safety Assessment were provided in a special data report /Andersson, 1999/. A similar report will be produced for the Safety Assessments during the Site Investigation phase.

3.5 Handling alternative models

All uncertainty cannot be handled or described as data uncertainty distributions. There may be a need to formulate alternative models. In principle, alternatives may both concern

- alternative geometrical framework (i.e. the geometry of deformation zones and rock domains, Figure 3-9),
- alternative descriptions (models such as DFN or SC – or parameter values) within the same geometrical framework.

There are several challenges, which needs to be handled while dealing with alternatives. In particular, it may be difficult for modelling teams to develop different alternative models in parallel. Furthermore, as models are used as input to the other models the total number of alternatives may become impractical to handle – ‘variant explosion’.

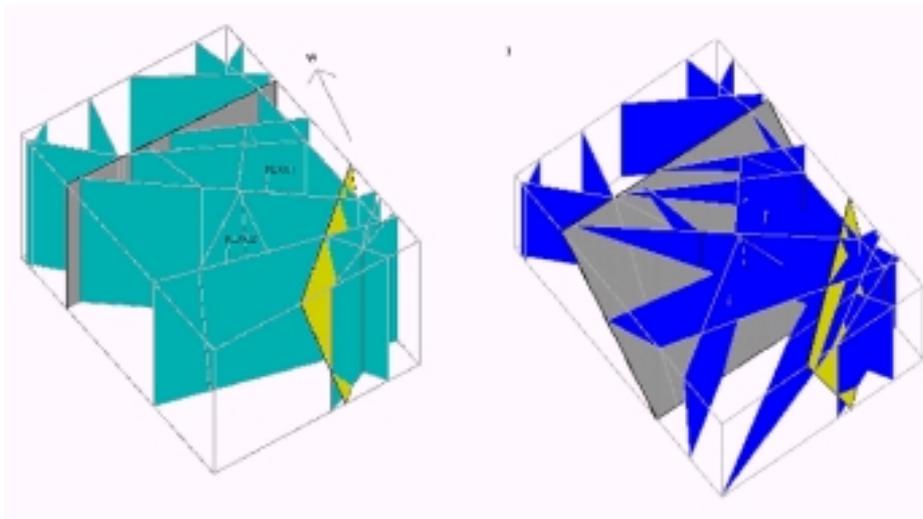


Figure 3-9. Alternatives may concern different geometrical frameworks.

How to develop different alternatives?

The level of information at the early stages of the site investigation clearly warrants the need to produce alternative descriptions. Still, in practice, maintaining several alternatives leads to a substantially increased workload. Furthermore, the distinction between alternative and updated version is not always easy to uphold. Insights gained in producing the first ‘alternative’ are hard to put aside when developing additional ones. Careful planning and a project commitment to produce alternatives are required.

All alternatives need not be equally probable. One way of producing alternatives may be to put different emphases on different aspects of the data – e.g. to only include hydraulically verified features or to include all radar reflectors etc. Another idea could be to consider different conceptual models of the site – e.g. assuming it likely (or not) to be many sub-horizontal zones in the volume etc.

Alternative model generation should be seen as a means for model development in general and as a means of exploring the confidence (see section 3.8). At least in early stages, when there is little information, it is evident that there will be several different possible interpretations of the data, but this may not necessitate that all possible alternatives are propagated through the entire analysis. It could be fruitful to develop a main alternative and a few side alternatives. When more information becomes available the subsequent testing and potential rejection of some alternatives may prove to be a rather convincing ‘track record’ on how the finally selected alternative(s) is selected. For example, in the SKI SITE-94 /SKI, 1996/ three different ‘alternatives’ to the Äspö structure model were presented and used as an illustration of uncertainty. However, examining the support for these alternatives demonstrated clear differences. While this could be criticised it also demonstrates that attempting alternative generation followed by later rejection of some alternatives could be an efficient means of arguing for the finally ‘selected’ alternative.

If possible, modellers should discuss also the ‘likelihood’ of the different alternatives, as this may be useful for subsequent risk analyses in the Safety Assessment. However, given the illustrative nature of the developed alternatives, such a ‘likelihood’ should not be seen as strict probabilities. Verbal descriptions or possibly ranking between alternatives is sufficient. In this context it is also necessary to remember the difference between the Site Descriptive Model and different analyses conducted by Safety Assessment or Rock Engineering. Within the uncertainty description provided by the Site Descriptive Model, Safety Assessment may modify alternatives or develop new alternatives. For example, Safety Assessment may see a need to explore the significance of an uncertain fracture zone or to explore different scaling rules of the rock mass parameters.

Handling ‘variant explosion’?

In theory the number of alternatives and variants to consider may be enormous, considering that e.g. the geometrical framework is used as input to the hydrogeological description, which in turn is used by the transport description. Furthermore, too many (possibly quite similar) alternatives may create a false impression of limited understanding. In reality the problem may be less acute considering the practical difficulties of even generating different alternatives. Nevertheless, a structured and motivated approach is needed to handle potential variant explosion, ensuring that important alternatives are not arbitrarily dropped.

Alternatives should illustrate the wealth of potentially different interpretations. Uncertainties in properties and even in e.g. orientation of fracture zones need not warrant alternative generation, but is rather handled by quantifying the uncertainty of the property estimates. Different alternatives should focus on clear differences in the geometrical framework and on clear differences on the description of the rock properties. An example of the latter is that the hydrogeological description includes both Stochastic Continuum (SC) and Discrete Fracture Network (DFN) representation of the conductive features of the rock.

It may also be worthwhile to consider whether different alternatives really would have different implications in subsequent analyses in Safety Assessment or Rock Engineering. However, this possibility could only be used with caution since the Site Descriptive Models will have many uses. Still, documented, feedback from Safety Assessment and Rock Engineering may be a way forward in selecting and omitting alternatives.

Well motivated and disciplined, integrated modelling, considering all data, is more important than developing a multitude of more or less realistic alternatives. But alternatives will be needed and the wealth of information, at least in the early stages of the Site Investigation, will not be sufficient to bind the interpretation to one model.

3.6 Input to scenario uncertainty

The Site Descriptive Models do not concern future external events. However, site specific conditions, for example regional boundary conditions or different indications of past evolution, could provide essential input to the scenario formulation in the Safety Assessment. The Site Descriptive Model need thus search for and document such conditions.

The geological evolution model provides a framework for the scenario analysis – even if the time scale of the geological evolution (1000 My) is several orders of magnitude larger than the time scale of interest for Safety Assessment.

Events potentially connected to previous glaciations may be of higher interests. This includes potential indications of neo-tectonic events, past shore level displacements and hydrogeochemical imprints of past water bodies and boundary conditions.

Understanding the past hydrogeological and hydrogeochemical evolution may imply an essential key to the confidence in the future predictions of this evolution. Also the confidence of the transport description may be enhanced by assessment of past transport phenomena at the site.

3.7 Conceptual uncertainty

SKB has collected its process understanding in a “process report” /SKB, 1999b/, first published as a supporting document to the SR 97 Safety Assessment /SKB, 1999a/. The process report will be updated, during the Site Investigation, as a part of the Safety Assessment activities.

The conceptual uncertainty in the Site Descriptive Model should be assessed and documented in the model description. The description could be both qualitative – a verbal description in the confidence of the applied conceptual model (see section 3.8 below) – and quantitative by formulating alternative models (see section 3.5 above).

Conceptual uncertainty is mainly an issue for Safety Assessment, rather than for Site Descriptive Modelling. Nevertheless, observations and uncertainty concerning the basic structure of the rock and on past and ongoing processes belong to the Site Description. Such conceptual uncertainties shall be discussed.

3.8 Confidence

The confidence in the descriptive model is essentially a qualitative entity. Still, judgement of confidence needs to be based on several specific analyses. For example:

- The method of interpretation is key to the confidence assessment. A similar and unbiased treatment of all different data and interpretations that explains several different observations enhances confidence.
- Consistency (i.e. no conflicts) between the different discipline model interpretations and with the geological evolution model enhances confidence.
- Data and data sources need to be quality assured according to issued manuals and procedures. Yet, this is a necessary but not a sufficient condition for confidence – the data also need to be properly understood! Also the users need to check the input data.
- Small estimated uncertainties and inability to produce many different alternative interpretations from the same database are indications of confidence – although no strict proof.
- Another indication of confidence is to what extent measurement results from late stages of the investigation compare well with previous predictions.

The latter point will also be important for discussing the potential benefit of additional measurements. Clearly, if new data compare well with previous prediction, the need for yet additional data may diminish.

It is also essential that the model descriptions can be used to explain current day conditions by the naturally ongoing processes considered being important. The distribution of the groundwater compositions should, for example, be reasonable in relation to rock type distribution, fracture minerals, current and past groundwater flow and other past changes. Such ‘paleohydrogeologic’ arguments may provide important contributions to confidence even if they may not be developed into ‘proofs’.

Developing confidence rests on a clear hypothesis testing and documented joint evaluation between the different disciplines. A related question is how to represent the varying degree of confidence. The following are examples of what should be considered during the course of the work:

- How is confidence affected by verification (or rejection) of previous predictions (i.e. earlier model versions)?

- How is confidence related to the information density? The confidence in a geological description is much governed by the overall geological understanding. Confidence in the description could be high even if there are few measurements if geological understanding is high (e.g. if there is a homogenous and evident geology), but could also be low, even with a 'wealth' of data, if the geological understanding is poor.
- Are there measurements or other tests, which could separate between alternatives and enhance confidence?

Confidence is to a large extent dependent on 'expert judgement'. This can not be directly quantified, but the procedures for making the judgements need to be transparently documented, making it possible for reviewers to assess the quality of the judgements made. It needs also be understood that modelling teams only can describe their own confidence. It is the traceable and logical description of how models are derived, how uncertainties are assessed and how this information influences the modellers understanding, which are the means for the reviewers to assess their confidence.

4 Concluding remarks

The strategy for integrated evaluation as described in the current document is not a strict and detailed instruction for how to carry out such a complex task. It rather provides some basic structure and principles to the modelling process and discusses particular issues and suggests means of addressing these. Clearly, during the course of the modelling work, challenges not anticipated here will arise and be resolved. The entire modelling process will be a learning process and the modelling strategy *must* therefore be *flexible* and *updated* accordingly.

Devotion and professionalism of the modellers are necessary quality factors. However, in addition the principles and procedures are needed for consistent handling of modelling matters throughout the Site Investigations and to ensure that different sites are handled equally. The strategy as outlined here should be one important instrument for assuring such consistency, but needs to be followed on by more detailed procedures and protocols ensuring that the strategy will in fact be followed.

5 References

- Andersson J, 1999.** SR 97: Data and Data Uncertainties, Compilation of Data and Evaluation of Data Uncertainties for Radio-nuclide Transport Calculations, SKB TR-99-09, Svensk Kärnbränslehantering AB.
- Andersson J, Christiansson R, Hudson J A, 2002a.** Site Investigations Strategy for Development of a Rock Mechanics Site Descriptive Model, SKB TR-02-01, Svensk Kärnbränslehantering AB.
- Andersson J, Berglund J, Follin S, Hakami E, Halvarson J, Hermanson J, Laaksoharju M, Rhén I, Wahlgren C H, 2002b.** Testing the Methodology for Site Descriptive Modelling. Application for the Laxemar area. SKB TR-02-19, Svensk Kärnbränslehantering AB.
- Berglund S, Selroos J-O, 2003.** Transport Properties Site Descriptive Model – Guidelines for Evaluation and Modelling. SKB R-03-09, Svensk Kärnbränslehantering AB.
- Follin S, Svensson U, 2002.** Groundwater flow simulations in support of the Local Scale Hydrogeologic Description developed within the Laxemar Methodology Test Project, SKB R-02-29, Svensk Kärnbränslehantering AB.
- Löfgren A, Brydsten L, Engqvist 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.
- Munier R, Hermanson J, 2001.** Metodik för geometrisk modellering. Presentation och administration av platsbeskrivande modeller (In Swedish: Methodology for geometrical modelling. Presentation and administration of site descriptive models). SKB R-01-15, Svensk Kärnbränslehantering AB.
- Munier R, Stanfors R, Stenberg L, Milnes A G, 2003.** Geological Site Descriptive Model – a strategy for the model development during site investigations. SKB R-03-07, Svensk Kärnbränslehantering AB.
- Rhén I, Follin S, Hermansson J, 2003.** Hydrogeological Site Descriptive Model – a strategy for the development during Site Investigations Rhén et al, SKB R-03-08, Svensk Kärnbränslehantering AB.
- SKB, 1999a.** SR 97 – Post-closure safety. Deep repository for spent nuclear fuel. Main Report (Volumes I and II). Svensk Kärnbränslehantering AB.
- SKB, 1999b.** SR 97 – Processer i förvarets utveckling, Underlagsrapport till SR 97, Svensk Kärnbränslehantering AB.
- SKB, 2000.** Geoscientific programme for investigation and evaluation of sites for the deep repository. SKB TR-00-20, Svensk Kärnbränslehantering AB
- SKB, 2001.** Site investigations: Characterisation methods and general execution programme , SKB TR-01-29, Svensk Kärnbränslehantering AB.

SKI, 1996. The SKI Deep Repository Performance Assessment Research Project SITE-94. SKI Report 96:36. Swedish Nuclear Power Inspectorate, Stockholm.

Smellie J, Laaksoharju M, Tullborg E-L, 2002. Site investigations. Strategy for the development of a hydrogeochemical site Descriptive model, SKB R-02-49, Svensk Kärnbränslehantering AB.

SSI, 1998. The Swedish Radiation Protection Institute's Regulations on the Protection of Human Health and the Environment in connection with the Final Management of Spent Nuclear Fuel and Nuclear Waste, SSI FS 1998:1, Swedish Radiation Protection Institute, Stockholm.

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