

Hydrogeochemical site descriptive model – a strategy for the model development during site investigations

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December 2002

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

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Preface

The aim of this exercise is to create a document with guidelines and a strategy for future site investigations, including groundwater sampling, hydrogeochemical evaluation and modelling and finally documentation, compiled from the information and experience gained over 20 years of SKB hydrogeochemical site investigations. Consequently, the major focus of this report is on sampling requirements, the step-wise sequence of evaluation and the iterative evolution of a Hydrogeochemical Site Descriptive Model, closely integrated with equivalent geological and hydrogeological site descriptive models.

The approach to hydrogeochemical site evaluation and modelling should not be bound strictly to what is stated as procedure here. This report should be considered a 'living document', allowing flexibility and change to accommodate unforeseen conditions encountered during the execution of site characterisations and the possible repercussions on the nature of the collected data and subsequent methodologies and interpretation.

Summary

The Swedish Nuclear Fuel and Waste Management Co (SKB) is responsible for the handling and final disposal of the nuclear waste produced in Sweden. In 2002, SKB commenced site characterisation investigations using deep boreholes at different sites. As an integral part of the planning work SKB has prepared a strategy to develop a Hydrogeochemical Site Descriptive Model; similar strategies have been developed for the other major geoscience disciplines. The objective of the strategy as presented in this report is that it should guide the practical implementation of evaluating hydrogeochemical data during Site Characterisation. It is also understood that further development, modification and updating of the strategy may be required as site investigations gain momentum.

Several of the requirements for developing a strategy leading to a Hydrogeochemical Site Descriptive Model are general to all the major disciplines involved in the overall modelling strategy. The main strategy requirements which are the focus of this report:

- are developed for needs connected to siting and building a KBS-3 type repository in crystalline rock,
- should be adapted to the iterative and integrated character of the Site Investigation and Site Evaluation programme,
- should allow full transparency of data gathering, management, interpretations, analysis and the presentation of results, and
- should make use of practical experience and observations from, for example, the SKB Äspö HRL site characterisation.

Major components, aims and scope

The Hydrogeochemical Site Descriptive Model combines a quantitatively-derived hydrogeochemical model (i.e. based on site measurements) and a qualitatively-derived hydrogeochemical model (i.e. more descriptive, process-oriented conceptual model). The main objectives of the Hydrogeochemical Site Descriptive Model 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 is based primarily on measurements of the groundwater composition but incorporates the use of available geological and hydrogeological site descriptive models. The description serves as the basis for possible hydrogeochemical simulations of the palaeohydrogeochemical evolution of the site and allows prediction of future changes.

The scope of the Hydrogeochemical Site Descriptive Model is:

- to understand the origin and evolution of the groundwater chemistry,
- to understand the influence of the surrounding lithological types on the groundwater chemistry,
- to understand the influence of the fracture mineralogy (through water/rock reactions) on the groundwater chemistry,
- to understand the influence of hydraulic mixing processes on the present groundwater chemistry,
- to understand the influence of hydraulic mixing processes on the past composition of the groundwater (i.e. palaeohydrogeochemistry),
- to allow assessment of future hydrogeochemical changes (i.e. forward predictions) at repository depths.

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

Sampling and analysis strategy

The SKB hydrogeochemistry programme is planned to fulfil two basic requirements:

1) to provide representative and quality assured data for use as input parameter values in calculating long-term repository safety, and 2) to understand the present undisturbed hydrogeochemical conditions and how these conditions will change in the future.

Parameter values for safety analysis include pH, Eh, S, SO₄, HCO₃, HPO₄ and TDS (mainly cations), together with colloids, fulvic and humic acids, other organics, bacteria and nitrogen. These values will be used to characterise the groundwater environment at, above and below repository depths. When the hydrogeochemical environment has been fully characterised, this knowledge, together with an understanding of the past and present groundwater evolution, should provide the basis for predicting future changes.

In the hydrogeochemical site investigation programme the number and location of the sampling points will be constrained by: a) geology (e.g. topography, overburden types, bedrock structures etc), b) hydrogeology (e.g. groundwater recharge/discharge areas, residence times), c) reliability (e.g. undisturbed vs disturbed groundwater chemical conditions), and d) resources (e.g. number and type of samples, and also available personnel, may be restricted by budgetary and schedule concerns). Naturally a balance is required between these constraints and the scientific aims of the programme. The constraints should never detrimentally affect the overall aim of providing sufficient and reliable scientific knowledge to describe adequately and accurately the hydrogeochemical conditions at the site.

In addition to these constraints, certain priorities have to be listed and addressed because of the size and complexity of the site investigation programme. Such priorities may be planned prior to field activities, whilst others will result from an on-going evaluation of

field activities and scientific or modelling needs under the direction of the SKB Site Analysis Team. This team will liaise closely with those responsible field personnel.

Based on past experience, identified priorities include:

- minimising groundwater contamination in the collected samples,
- sampling end member groundwater conditions (e.g. recharge/discharge conditions, or high/low topographic locations and shorelines) to define important boundary conditions for hydrogeochemical and hydrodynamic modelling,
- sampling of end member water compositions rather than groundwater mixtures,
- sampling groundwaters close to repository depth,
- understanding the spatial variation of chemical parameters closely integrated with hydrogeological conditions,
- measuring a large number of spatially strategic points (including time series measurements) distributed vertically and laterally over a large area,
- simultaneous sampling from many boreholes to produce accurate, time-related 3D interpolated ‘snap shots’ of important groundwater parameters.

Sampling of low permeable rocks and fracture zones of low transmissivities will be allocated greater priority.

Some five classes of chemical analyses are available to characterise the collected groundwater samples. The choice of class will depend on the hydrogeochemical information required, the location to be sampled and the sampling method used.

The major hydrogeochemical output data from a 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 may be related broadly to three major site subdivisions, i.e. surface, near-surface and sub-surface. Alternative subdivisions (simplified or more rigorous) may be considered depending on the complexity of the site under investigation and the availability of data. Hydraulic data, for example groundwater flow rates and hydraulic gradient directions, and geological data, for example variations in lithology, fracture frequency and fracture mineral chemistry, will play an important role in establishing such divisions.

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. This will include emphasis on identifying the major chemical processes through modelling water/rock reactions and also modelling the mixing effects of different groundwater end members. Studies will involve not only present-day hydraulic conditions, but will also attempt to trace past conditions using palaeo-evidence from groundwaters and fracture minerals.

Model evolution and end-product

During the course of the site characterisation, the Hydrogeochemistry Site Descriptive Model will undergo a continuous and step-wise updating as additional data become available, resulting in a series of model iterations based on the Initial Site Investigation (ISI) stage (Model version 1) and model iterations based on the Complete Site Investigation (CSI) stage (Model version 2).

The various stages involved in the evaluation and interpretation of the hydrogeochemical data, and the interrelationships between the different stages are outlined in Figure A. The sequence illustrated can be applied at different junctures of the site investigations, for example, initially during the ISI investigation stage (e.g. version 1 as illustrated in Figure A) and later during the CSI investigation stage (version 2) when additional and more comprehensive data become available. Once again, depending on the complexity of the site, additional iterations may have to be considered. These evaluations will result in a series of Hydrogeochemical Site Descriptive Model versions (e.g. version x.x in Figure A), each version representing the input of additional and new data with a corresponding updating and modification of the previous model. These iterations will lead eventually to a final Hydrogeochemical Site Descriptive Model. Based on this final model, sub-models describing the surface, near-surface and sub-surface hydrogeochemical environments also may be constructed. The number, type and complexity of the sub-models will be determined when the nature of the site conditions become more apparent during the site investigations.

The final version of the Hydrogeochemical Site Descriptive Model should represent a site-scale hydrogeochemical interpretation fully integrated with the corresponding final site descriptive versions of the geological and hydrogeological models. This final model version should show clearly:

- the major lithological and structural units comprising the site,
- the major groundwater flow directions (and minor flow directions if possible),
- the relationship of chemistry (i.e. mixing of end members; chemical reactions etc) to these major hydraulically conducting pathways (i.e. Hydraulic Conducting Domains; HCDs),
- a clear indication of the groundwater types representative of the main hydraulic rock mass units (i.e. Hydraulic Rockmass Domains; HRDs) characterised by fractures (fracture zones) of lower transmissivities,
- an indication, if possible, of the chemistry of the rock matrix pore space fluid/groundwater (i.e. confined to rock units of lowest permeability).

Such information will also help to establish the input boundary conditions for the numerical hydrodynamic models.

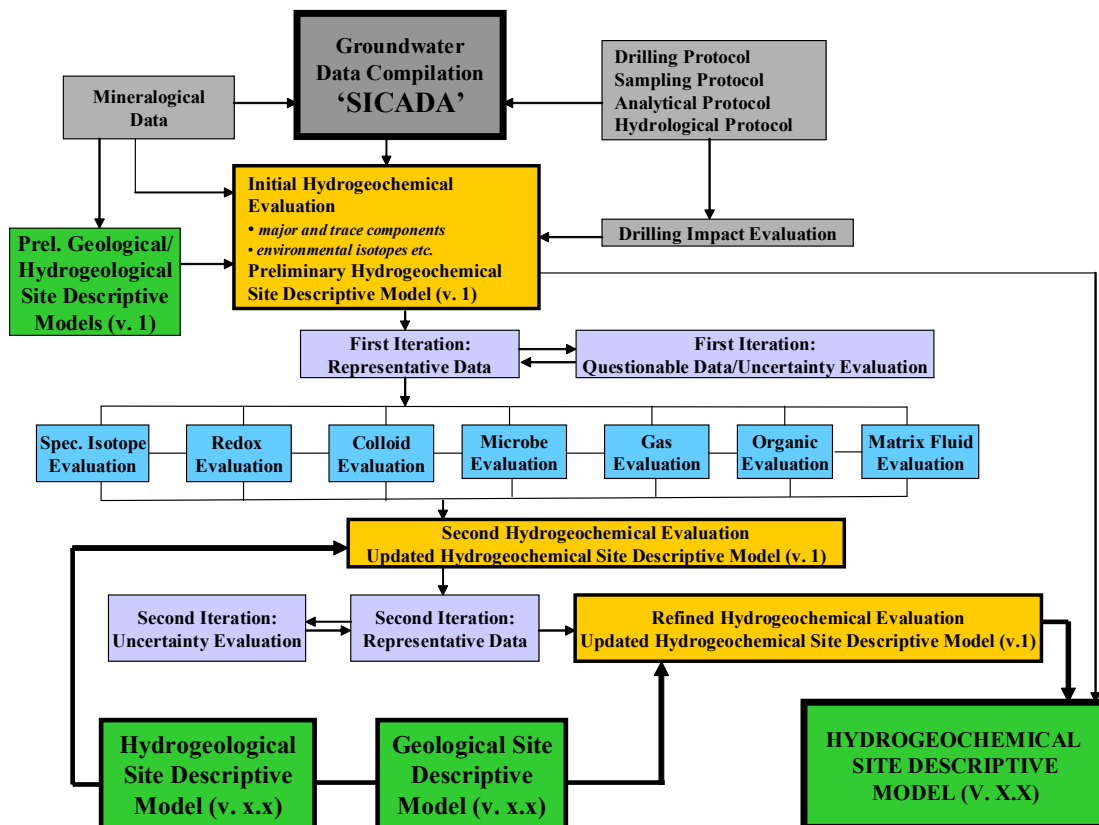


Figure A. Flowchart showing the step-wise approach of integration and development involved in the hydrogeochemical evaluation of the Initial Site Investigation (ISI) stage to produce a Hydrogeochemical Site Descriptive Model. Yellow font indicates the major stages in the hydrogeochemical evaluation.

Management of uncertainties

At every phase of the hydrogeochemical investigation programme, for example drilling, sampling, analysis, evaluation and modelling, uncertainties are introduced which have to be accounted for, addressed fully and clearly documented to provide confidence in the end result, whether it will be the site descriptive model or repository safety analysis and design. The uncertainties involved in constructing a site descriptive model include: a) conceptual uncertainty, b) data uncertainty, c) spatial variability of data, d) chosen scales, e) degrees of confidence, and f) error, precision and accuracy. When possible, these uncertainties have been addressed systematically at each step of the hydrogeochemical evaluation and interpretation process.

Documentation

Documentation will be in the form of a written document together with a detailed record of the various steps fulfilled in the construction of the Hydrogeochemical Site Descriptive Model. These details are contained in an overall activity plan which defines the major aims, the steps involved in their achievement, the methodology to be employed, the expected output data and the time schedules to be met. Activities prior, during and subsequent to execution of the model construction will be documented, including when deviation from the activity plan has occurred.

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1 Introduction

In the event of canister breakdown and penetration of groundwater, the solubility and mobilisation of potentially dangerous radionuclides and their subsequent transport to the biosphere will be greatly influenced by the groundwater chemistry. It is not only the chemistry and hydrodynamics of the groundwater at repository depths that are important, but also the variation in groundwater chemistry at progressively shallower depths along the discharging groundwater flow paths. Thus, hydrogeochemically characterising a candidate site for the disposal of radioactive waste will include detailed studies of groundwaters sampled from the surface and overburden (inclusive of sea-bottom sediments if present), together with the near-surface and sub-surface bedrock environments.

Furthermore it is not only present-day conditions that should be given priority. To help establish time-dependent boundary conditions for forward predictions of hydrochemical stability within the repository environment, an understanding of the past evolution of deep groundwater systems (known as palaeohydrogeology) is essential. The fact that palaeohydrogeology has not been specifically emphasised as a disciplinary study in this report is not that it has been ignored, but traditionally at SKB it has been included naturally as an integral part of the hydrogeochemical studies.

The major objectives of the hydrogeochemical site characterisation studies, based on /SKB, 2001/, are:

- to characterise the undisturbed groundwater chemistry and describe its origin, distribution and development in the bedrock as a function of depth and lateral extent,
- to focus on those physico-chemical parameters important for safety analysis and forward predictions (e.g. pH, Eh, chloride, sulphide, colloids etc),
- to establish the presence or otherwise of dissolved oxygen in groundwaters at repository depths.

The scope of such studies is:

- to sample undisturbed/representative groundwaters from the surface, near-surface and sub-surface environments (e.g. from precipitation, lakes, streams, springs, shallow overburden screens, intermediate to deep percussion and rotary-drilled boreholes and sediment (including sea-bottom sediments) porewaters etc),
- to measure those major ions, trace elements and environmental isotopes (and other related parameters such as gas contents and populations of colloids, microbes and organics) necessary to characterise the different groundwater types and to establish their origin and evolution,
- to use these data to: a) describe present-day undisturbed groundwater conditions, b) estimate palaeo-conditions which may reflect past climatic events (e.g. glacial effects), c) estimate future changes in groundwater conditions during the lifespan of the repository (i.e. short-term construction and operational phases and the long-term post-closure phase) and, d) provide realistic input chemical parameters to repository safety and performance analyses.

The primary data resulting from these studies, both measured and calculated values, will be stored in the SKB geoscientific database SICADA (Site ChAracterisation DAtabase) /SKB, 2000/. To judge the reliability of this information and to evaluate its use in the design and safety assessment of a repository, it must be interpreted and presented in a final site descriptive model. This model incorporates a description of the geometry and the various properties of the site (e.g. the geology, hydrogeology and hydrogeochemistry). The geometric bedrock model (i.e. the Rock Visualisation System – RVS) will be based mainly on geological information, but information from the other disciplines also will be included /SKB, 2000/.

During the course of the site characterisation, the overall site descriptive model undergoes a continuous and stepwise updating as additional data become available, resulting in a series of model versions which provide input into each stage of repository design and safety assessment. An integral part of this overall model evaluation is based on input from the hydrogeochemical data produced at the different steps and scales (i.e. regional, local and block scale) conducted during the site investigation programme. For example, a hydrogeochemical site descriptive model is constructed at every step and each model is successively modified and updated until a final hydrogeochemical site descriptive model for the site is produced. This model, together with similar descriptive models from, for example, the geological and hydrogeological investigations, forms the basis of the final site descriptive model.

Based on the compiled, evaluated and modelled hydrogeochemical data from the site characterisation, which will include an understanding of those parameters relating to long-term hydrogeochemical stability, the next stage is to decide how these data can be used as direct input to assess the future safety and performance of a repository and in what form should these data be presented? Possibilities include: a) 3D visualisation in space, b) glacial scenario development, and c) suitable range of groundwater compositions.

The aim of this document is to use the information and experience gained over 20 years of SKB hydrogeochemical site investigations and focus this knowledge to provide a strategy for the evaluation and modelling of hydrogeochemical data resulting from present and future site investigations. The results of this knowledge are detailed in several reports /e.g. SKB, 2000; 2001/ and the step-wise sequence of evaluation and site descriptive modelling, outlined in Figure 1-1, is a major focus of the report. Where relevant, aspects of the evaluation exercise conducted at the Laxemar site ('Testing the methodology for site descriptive modelling: Application for the Laxemar area' /Andersson et al, 2002/) have been incorporated. The ultimate aim is to provide sufficient background information to form a basis for the SKB site characterisations.

This document addresses both the 'Guidelines' and 'Methodology' related to hydrogeochemical site characterisation leading to a hydrogeochemical site descriptive model. However, it should be emphasised that the recommended approach to hydrogeochemical site evaluation and modelling should not be bound strictly to what is stated here. This report should be considered a 'living document', allowing flexibility and change to accommodate unforeseen conditions encountered during the execution of site characterisations and the possible repercussions on the nature of the collected data and subsequent methodologies, interpretation and modelling.

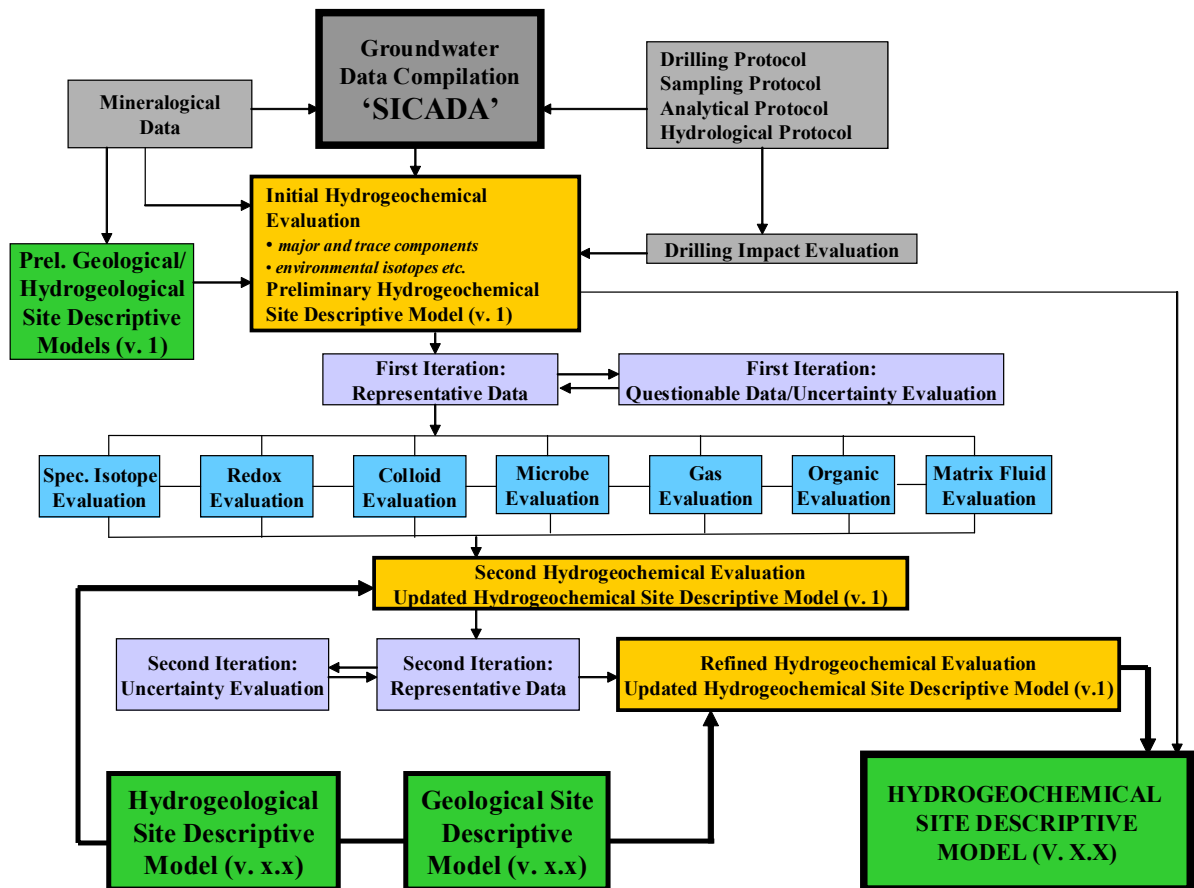


Figure 1-1. Flowchart showing the step-wise approach of integration and development involved in the hydrogeochemical evaluation of the Initial Site Investigation (ISI) stage to produce a hydrogeochemical site descriptive model. Yellow font indicates the major stages in the hydrogeochemical evaluation.

2 Development of hydrogeochemical site descriptive models

2.1 Objectives and scope

The Hydrogeochemical Site Descriptive Model combines a quantitatively-derived hydrogeochemical model (i.e. based on site measurements) and a qualitatively-derived hydrogeochemical model (i.e. more descriptive, process-oriented conceptual model). The main objective of the Hydrogeochemical Site Descriptive Model is 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 is based primarily on measurements of the groundwater composition but also incorporates the use of available geological and hydrogeological descriptive models. The description also serves as the basis for possible simulations of the palaeohydrogeochemical evolution of the site and also to predict future changes /SKB, 2000/.

The scope of the Hydrogeochemical Site Descriptive Model is to understand:

- the origin and evolution of the groundwater,
- 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. palaeohydrogeology),
- future hydrogeochemical changes (i.e. forward predictions) at repository depths.

Furthermore, together with hydrogeological modelling, the Hydrogeochemical Site Descriptive Model should establish the basis for predicting short-term (some tens of years) changes in groundwater chemistry resulting from repository excavation and during open operational conditions.

2.2 Model versions

2.2.1 General

As mentioned in Chapter 1, primary data from the different site investigations are interpreted, analysed and presented in a final site descriptive model, and the objective of this model is to provide a description of the site that can be used for the design and safety assessment of a repository. The model is three-dimensional consisting of different geometric units in the bedrock and overburden. These units are determined by the geometry of the fracture zones and the lithological/overburden distribution. For each bedrock geometric unit the geological conditions are described together with the mechanical, thermal, hydraulic and hydrogeochemical properties and also those properties relevant to evaluating radionuclide transport /SKB, 2000/.

During the course of the site characterisation, the overall site descriptive model undergoes a continuous and step-wise updating as additional data become available, resulting in a series of model versions. In addition, a step-wise sequence of model construction, modification and evolution for each of the bedrock properties also results in a series of model versions.

These different model versions fall under the following categories:

- Model version 0 (based on the Feasibility Study (FS) stage).
- Model version 1 (based on the Initial Site Investigation (ISI) stage).
- Model version 2 (based on the Complete Site Investigation (CSI) stage).

With respect to hydrogeochemistry, a brief description of each model version is given below covering the rationale and the main input and output parameters; these details are further illustrated in Table 2-1. Note that Model version 0 is not represented in Table 2-1 or included in the hydrogeochemical site characterisation guidelines outlined in section 5.2 since it represents the Feasibility Study stage and not the site investigation stages proper. However it is included under section 2.2.2 for completeness.

2.2.2 Model version 0

This model input is based on the Feasibility Study stage and for the hydrogeochemical investigations mostly comprises a compilation of surface and near-surface groundwater data mainly obtained from the well archives of the Geological Survey of Sweden. Additional input is gathered from existing hydrogeochemical and hydrogeological knowledge of earlier site investigations. By combining all available information it is possible to construct a generalised descriptive model of the site to be investigated.

Input data

Input data comprises:

- geographic location (coastal vs inland site),
- topographical data,
- areas of groundwater recharge/discharge,
- surface/near-surface groundwater hydrochemical data (lakes, streams, springs, dug and drilled wells etc),
- hydrogeochemical evolution; present and past (data and experience from existing site investigations at similar geographic and topographic locations).

Table 2-1. Site investigation stages and components involved in the evolution of the Hydrogeochemical Site Descriptive Model

Input Data	Additional Input	Output Data	Product
<u>ISI Stage</u>			
Precipitation Streams Lakes/Sea Springs *Dug and drilled wells *Percussion boreholes (10–20) Sediment porewater Hydrochemical monitoring ⁺ Percussion boreholes ^{o+} Cored boreholes Fracture mineralogy	Geological Model (version 1) Hydrogeological Model (version 1)	Description of groundwater system (regional and local scales) Recharge/discharge areas Identification of major groundwater types Hydrochemical characterisation (e.g. redox; residence times) Spatial variation of chemical components Major chemical reactions	Hydrogeochemical Site Descriptive Model (version 1) Siting of 1–2 hydrogeochemical boreholes Planning of CSI stage
<u>CSI Stage</u>			
⁺ Percussion boreholes ^{o+} Cored boreholes Fracture mineralogy Hydrochemical monitoring	Geological Model (versions 2.1, 2.2..2.x etc) Hydrogeological Model (versions 2.1, 2.2..2.x etc)	Broad understanding of the site hydrogeology/ hydrogeochemistry, to repository depth and below (e.g. groundwater distribution, chemistry, mixing, reactions, residence times etc) (regional, local and block scales) Hydrochemical parameters, e.g. for transport modelling, long-term engineered barrier design, safety analysis etc	Hydrogeochemical Site Descriptive Model (versions 2.1, 2.2..2.x etc)

^o sampling during drilling; ⁺ sampling after drilling

Evaluation of data

Evaluation of data should lead to:

- a lateral and vertical extrapolation of major groundwater flow directions based on topography and possible hydrogeochemical indications of recharge/discharge areas,
- a lateral and vertical extrapolation of hydrogeochemical variations based on regional hydrogeology and experience from other geographically compatible site investigations,
- a possible palaeohydrogeochemical evaluation based on the above-mentioned points and experience from geographically compatible site investigations.

Output data

Evaluation of data should produce:

- a generalised site descriptive model of present major groundwater flow directions, potential areas of recharge/discharge and expected major variability of groundwater chemistry,
- a generalised palaeohydrogeochemical evolution of the site since the last glaciation /e.g. Laaksoharju et al, 1999a/.

2.2.3 Model version 1

Model version 1 essentially represents the Initial Site Investigation (ISI) stage resulting in hydrogeochemical data from surface and near-surface locations, and limited data from deep bedrock locations (Table 2-1). The ISI stage initially provides a spatial distribution of the variation of the major groundwater chemical components to facilitate the siting of 1–2 prioritised boreholes for hydrogeochemical studies, and later provides the basis for planning the campaign for the following Complete Site Investigation (CSI) stage.

Modelling will be carried out in two parts; the first part based on the initially derived data, and the second part representing an updated and modified model version as more data, particularly from the 1–2 prioritised hydrogeochemical boreholes, become available.

Input data

Input data comprises:

- sampling and analysis of groundwaters from surface and near-surface locations (including percussion boreholes),
- sampling and analysis during the drilling of core-drilled boreholes, including the 1–2 prioritised, deep boreholes (~ 1000 m) devoted to hydrogeochemical studies,
- additional hydrogeochemical data obtained from all borehole types:
 - pump tests,
 - downhole hydrochemical logging,
 - restricted sampling and analysis from isolated borehole sections.

Evaluation of data

Evaluation of data should lead to:

- identifying/confirming areas of groundwater recharge and discharge,
- identifying major groundwater types and the general effects of chemical reactions,
- possibly identifying the general effects of microbial processes on the hydrochemistry.

Output data

Evaluation of data should produce:

- a regional description of the groundwater system,
- a qualitative Hydrogeochemical Site Descriptive Model (version 1; see Figure 1-1) showing:
 - present major groundwater flow directions,
 - potential areas of recharge/discharge,
 - major groundwater types and their spatial distribution,
 - variability of groundwater chemistry based on mixing processes and hydrogeochemical reactions,
- a qualitative palaeohydrogeochemical interpretation of the site since the last glaciation,

2.2.4 Model version 2

The Complete Site Investigation (CSI) stage entails the complete chemical characterisation of the deeper groundwater systems /SKB, 2001/. Additional data to those used to construct Model version 1 will result from logging, sampling and analysis of new percussion and core-drilled boreholes, and long-term hydrochemical monitoring and resampling from existing boreholes. Together, these supplementary data will be used to update and modify Model version 1 to Model version 2 (see Table 2-1).

The deep groundwater data from repository depths will be used ultimately as direct input to evaluate: a) the long-term stability of individual engineered barriers, and b) the long-term performance and safety of the complete repository system.

Since the drilling programme will probably be carried out in stages, each drilling stage will involve a certain number of boreholes (probably 3–5), and hydrogeochemical characterisation at each stage will result in a different model version which will be an updated version of the preceding model. This will result in a series of site descriptive model versions such as Model version 2.1, 2.2, 2.3 ...2.x etc (Table 2-1).

2.3 Final Hydrogeochemical Site Descriptive Model

The final version of the Hydrogeochemical Site Descriptive Model, reflecting the culmination of model evolution from version 1 through version 2.x to a final version x.x, will represent therefore a site-scale hydrogeochemical interpretation fully integrated with the corresponding final site descriptive versions of the geological and hydrogeological models. This final Hydrogeochemical Site Descriptive Model version x.x should show clearly:

- the major lithological and structural units comprising the site,
- the major groundwater flow directions (and more minor flow directions if possible),
- the relationship of chemistry (i.e. mixing of end-members; chemical reactions etc) to these hydraulically conducting pathways (i.e. Hydraulic Conducting Domains; HCDs),
- a clear indication of the groundwater types representative of the main hydraulic rock mass units (i.e. Hydraulic Rockmass Domains; HRDs) characterised by lower transmissivities,
- an indication, if possible, of the chemistry of the rock matrix pore fluid/groundwater (i.e. rock units of lowest transmissivities).

Such information will also help to establish the input boundary conditions for the numerical hydrodynamic models.

3 Sampling, analysis and output data

3.1 General

As detailed in Chapter 2, two site investigation phases are planned: An Initial Site Investigation (ISI) phase and a Complete Site Investigation (CSI) phase. These two phases are preceded by a Feasibility Study (FS) and followed by a Detailed Characterisation (when the final candidate site is selected; the DC phase is not addressed in this report. With respect to the hydrogeochemistry programme, the ISI phase will provide most of the data from surface-based sampling and analysis, and the CSI phase from subsurface sampling and analysis.

The hydrogeochemistry programme /SKB, 2001/ is planned to fulfil two basic requirements: 1) to provide representative and quality assured data for use as input parameter values in calculating long-term repository safety, and 2) to understand the present undisturbed hydrogeochemical conditions and how these conditions will change in the future. Parameter values for safety analysis include pH, Eh, S, SO₄, HCO₃, HPO₄ and TDS (mainly cations), together with colloids, fulvic and humic acids, other organics, bacteria and nitrogen. These values will be used to characterise the groundwater environment at, above and below repository depths. When the hydrogeochemical environment has been fully characterised, this knowledge, together with an understanding of the past and present groundwater evolution, will provide the basis for predicting future changes.

3.2 Sampling and analysis strategy

3.2.1 General

In the hydrogeochemical site characterisation programme the number and location of the sampling points will be constrained by:

- **Geology**, meaning that the topography, overburden types and bedrock structures determine the best possible sampling locations at the surface or in the bedrock.
- **Hydrogeology**, meaning that the sampling locations have to include groundwater recharge/discharge areas and intermediate- to long-term residence time groundwater volumes in the bedrock and overburden.
- **Reliability**, meaning that the sampling programme needs to reflect the undisturbed groundwater chemical conditions and its natural temporal and spatial variability, and to describe the degree of sampling disturbances at the site and especially at repository depth.
- **Resources**, meaning that the number and type of samples may be restricted by budgetary and schedule concerns; budgetary restrictions may, in turn, influence the availability of personnel.

Naturally a balance is required between the above-listed constraints and the scientific aims of the programme. The constraints should never detrimentally affect the overall aim of providing sufficient and reliable scientific knowledge to describe adequately and accurately the hydrogeochemical conditions at the site.

3.2.2 Rationale and strategy

The groundwater sampling rationale and strategy is based on deriving adequate information to: a) characterise the groundwaters at repository depths, and b) describe the past and present origin and evolution of the groundwater system. The question is how best to achieve the amount and quality of analytical data required to accomplish these requirements. For example:

- Which locations will provide the most useful data?
- How many samples are required to be collected and over what time-scales (i.e. hours, days, months or years)?
- Frequency of sampling (i.e. regular or sporadic)?
- What level/quality of data is required?
- What level/quality of data is practically possible, given:
 - the intended use of the data?
 - the sampling locations selected?
 - the available sampling methods to be used?
 - the time constraints imposed by the overall site characterisation programme?

The step-wise planning of the ISI and CSI investigation phases over timescales of months to years has several advantages for the hydrogeochemical programme. For example, it allows hydrogeochemical sampling/monitoring to:

- establish different groundwater types/end-members,
- establish the variation in groundwater chemistry from fractures (zones) of different hydraulic and geological character, thus providing information and support, for example, for groundwater mixing and delineation of major flow directions,
- establish open borehole circulation trends,
- establish seasonal variations.

However, certain disadvantages are also present and sometimes unavoidable. For example, since subsurface downhole groundwater sampling in particular can be very sensitive to disturbances (drilling, borehole logging, pumping etc), occasions arise when a chosen sampling methodology (e.g. sampling during drilling) does not permit reliable analysis, or that only a limited number of chemical parameters can be determined. Time constraints can also result in inadequate or incomplete sampling. Consequently, within the ISI and CSI investigation stages several classes of sampling and analysis have been identified which reflect in some cases the hydrogeochemical information required and in other cases the drawbacks/difficulties of various sampling methodologies employed to achieve this information.

Five different classes have been recognised /SKB, 2001/:

- **Class 1:** Simple sampling during time-series monitoring to establish groundwater stability (i.e. constant composition achieved with respect to the environment).
- **Class 2:** Simple sampling to classify major groundwater types.
- **Class 3:** Simple sampling to identify major groundwater components (excluding redox parameters).
- **Class 4:** Comprehensive sampling for complete groundwater chemical characterisation.
- **Class 5:** Comprehensive sampling for complete groundwater chemical characterisation including specialised analyses.

Table 3-1. Description of SKB's chemistry classification for groundwater sampling and analysis /SKB, 2001/

Class	Description
Class 1:	<p>Simple sampling for verification of temporal stability – Electrical conductivity, pH, uranine*, temperature</p>
Class 2:	<p>Simple sampling for type classification – Electrical conductivity, pH, Cl, HCO₃, uranine*, temperature</p> <p>Options: a, b – a = Archiving of frozen samples – b = δ²H, ³H, δ¹⁸O</p>
Class 3:	<p>Simple sampling for determination of main components (not redox) – Electrical conductivity, pH, Cl, HCO₃, SO₄, Br, uranine*, temperature, cations (except Fe, Mn) and SO₄ analysed as sulphur with ICP-AES</p> <p>Options: a, b, c, d – a = Archiving of frozen samples – b = δ²H, ³H, δ¹⁸O – c = δ³⁴S (in SO₄), δ³⁷Cl, δ⁸⁷Sr, δ¹¹B – d = ¹⁴C, δ¹³C</p>
Class 4:	<p>Extensive sampling for complete chemical characterisation – Electrical conductivity, pH, Cl, HCO₃, SO₄, Br, uranine*, temperature, DOC, cations** and SO₄ (analysed as sulphur with ICP-AES) – δ²H, ³H, δ¹⁸O – HS⁻, NH₄ – Archiving of acidified and unpreserved frozen samples</p> <p>Options: e – e = NO₂, NO₃ and/or NO₂+NO₃, PO₄, F⁻, I⁻</p>
Class 5:	<p>Extensive sampling for complete chemical characterisation including special analyses – Electrical conductivity, pH, Cl, HCO₃, SO₄, Br, uranine*, temperature, DOC, cations** and S (analysed as sulphur with ICP-AES) – δ²H, ³H, δ¹⁸O – F⁻, I⁻ – HS⁻, NH₄, NO₂, NO₃ and/or NO₂+NO₃, PO₄ – Archiving of acidified and unpreserved frozen samples</p> <p>Options: c, d, f, g, h, i, j, k, l, m – c = Isotopes δ³⁴S (i SO₄), δ³⁷Cl, δ⁸⁷Sr, δ¹¹B – d = ¹⁴C, δ¹³C – f = Isotopes ²²⁶Ra, ²²⁸Ra and ²²²Rn – g = U and Th isotopes – h = Trace metals (ICP-MS, AAS and/or INM)*** – i = Dissolved gas (including δ¹⁸O, δ¹³C, ³He/⁴He), bacteria – j = Colloids – k = Humic and fulvic acids – l = pH and Eh measurements on-line</p>

* Determined only when uranine is used as a marker for drilling water (flushing water).

** Cations: Na, K, Ca, Mg, Fe, Mn, Li, Sr + Si.

*** Trace metals: U, Th, lanthanoids, heavy metals or own choice.

These classes and the chemical parameters measured, presented in more detail in Table 3-1, are applied at selected stages throughout the ISI and CSI investigation phases depending on the hydrogeochemical information required, the location to be sampled and the sampling method used.

3.2.3 Priorities

Because of the size and complexity of the site investigation programme, certain priorities have to be listed and addressed. Such priorities may be planned prior to field activities, whilst others will result from an on-going evaluation of field activities and scientific or modelling needs under the direction of the *SKB Site Analysis Team*. This group will liaise closely with those responsible field personnel.

Based on past experience, identified priorities and how they may be addressed are outlined below:

- To minimise groundwater contamination in collected samples is of high priority. To better control the volume of water entering or leaving the borehole sections prior to sampling, a DIS (Drilling Impact Study) will be carried out immediately when a borehole is drilled /Gurban and Laaksoharju, 2002/. Here the foreign groundwater volumes entering/extracted from the various fracture zones (i.e. comprising spiked flushing water and unspiked formational groundwaters) will be modelled during: a) drilling, b) subsequent borehole activities, c) sampling occasions, and c) the lifespan of the borehole. The accuracy of the modelling can be checked against field data, for example from sampling during drilling and from the standard groundwater sampling programme. The advantage with this approach is that the influence of the unspiked formation groundwater volumes (in contrast with the spiked flushing water volumes which are more easily assessed) on the undisturbed groundwater conditions can be modelled. This will help to plan the appropriate pumping period prior to sampling from packed-off borehole sections and will increase confidence in the representativeness of the collected samples.
- At the surface, samples reflecting hydrodynamic conditions such as recharge/discharge, or high/low topographic locations and shorelines have high priority because they provide important boundary conditions for the hydrogeochemical and hydrodynamic modelling exercises.
- Sampling close to the repository depth has high priority.
- Sampling of extreme water compositions has a higher priority than samples reflecting groundwater-mixtures between two or more extreme groundwater types.
- On occasions, priority is given to understand the wider site scale implications of the groundwater properties associated with groundwater types rather than focussing on problems associated with sampling or analyses of individual samples.
- To understand the origin and evolution of the groundwater system requires a greater knowledge of the spatial variation of chemical parameters (rather than specific, and restricted high quality data) and a close integration (and interpretation) with the hydrogeological conditions. The priority is therefore on obtaining a large number of measurement points (including time series measurements) distributed vertically and laterally over a large area and the data need not be the most representative.

- High quality groundwater data for specialised studies (see section 5.2.3) will be limited mostly to the prioritised hydrogeochemical boreholes. Some priority should be given for limited additional sampling locations of strategic importance when the site groundwater system is better characterised.
- When monitoring, simultaneous sampling from many borehole locations has higher priority than random sampling or detailed long-term sampling of individual boreholes. This strategy aims at producing accurate 3D interpolated ‘snap shots’ in time of important groundwater parameters such as Eh, pH, Cl, HCO₃, SO₄, saturation indexes and mixing proportions. This information can be used, for example, to judge chemical stability, to integrate with hydrogeology, or as a measure of disturbance from field activities. Several (at least 4) ‘snap shots’ will be produced annually to reflect undisturbed conditions, seasonal variations, long-term changes or changes due to field activities.
- Groundwaters from fractures of low transmissivity ($T = 10^{-11} - 10^{-9} \text{ m}^2 \text{ s}^{-1}$) and rock matrix or interconnected pore space groundwaters/fluids ($T = 10^{-14} - 10^{-12} \text{ m}^2 \text{ s}^{-1}$) will be prioritised since deposition of spent fuel will be restricted to rock volumes of low permeability.

3.3 Output data

The major hydrogeochemical output data from a 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),
- populations of colloids and microbes.

These data will result from a combination of surface sampling, downhole sampling of open boreholes and predetermined isolated borehole sections, and laboratory leaching/diffusion experiments of the rock matrix. Downhole long- and short-term hydrochemical monitoring also will provide very useful data. Furthermore, since groundwater chemistry and its interpretation is very much dependent on the bedrock geology and the hydraulic properties of the bedrock, close integration with these disciplines is essential at all stages.

The hydrogeochemical output data may be related broadly to three major site subdivisions, i.e. surface, near-surface and sub-surface. Alternative subdivisions (simplified or more rigorous) may be considered depending on the complexity of the site under investigation and the availability of data. Hydraulic data, for example groundwater flow rates and hydraulic gradient directions, and geological data, for example variations in lithology, fracture frequency and fracture mineral chemistry, will play an important role in establishing such divisions. Common to the near-surface and sub-surface divisions will be hydrogeochemical data from low transmissive fractures.

3.3.1 Surface information

This information will result mostly from the ISI stage of the site investigation programme where surface-based studies will contribute most to the available data. The objective is to establish the recharge/input water chemistry into the overburden and near-surface bedrock groundwater environments. Moreover, such information helps to provide some of the important initial and boundary conditions for subsequent hydrogeochemical and hydrodynamic model calculations.

Output data covers sampling and analysis of:

- precipitation (Class 3),
- waters from lakes and streams (Class 3),
- seawater (Class 5).

These data will supplement, for example, archive data from the Geological Survey of Sweden and other compiled data used in the Feasibility Study phase.

3.3.2 Near-surface information (~ 100 m)

This information will result mostly from the ISI stage and also will supplement archived well data from the Geological Survey of Sweden and other compiled data used in the Feasibility Study phase. This near-surface environment, comprising the transition of overburden (including lake or sea-bottom sediments) to the upper bedrock (i.e. biosphere/geosphere transition), is hydrogeochemically one of the most important reaction zones which ultimately determines the major input of critical groundwater physico-chemical properties (e.g. pH, Eh, HCO₃, SO₄ etc) to greater depths in the bedrock. Such a sampling campaign may also help to demarcate areas of recharge/discharge and the position of the redox boundary.

A depth of approximately 100 m has been allocated to this zone; this is based on the probability of local hydraulic gradients which in some cases may facilitate groundwater recharge to greater depths than the overburden/upper bedrock transition environment. The depth extent of this near-surface zone will therefore be very irregular and dependent on the number, extension and hydraulic character of vertical to sub-vertical fracture systems in the bedrock, and also the potential short-circuiting of these systems by intersecting sub-horizontal hydraulically active fractures.

Output data covers sampling and analysis of:

- springs (Class 3),
- wells (dug and drilled types; approximately three selected for 2-year seasonal monitoring; Class 3),
- shallow piezometric soil screens (several metres) in the overburden (some locations selected for 2-year seasonal monitoring; Class 5),
- sediment pore water (lake and/or sea bottom sediments); analytical class chosen will depend on the volume of extracted pore water obtained,
- early tube logging/sampling (50 m sections) of open percussion boreholes (10–20 drilled to approx. 150–200 m) (Class 3),
- strategic isolated sampling points in the percussion boreholes (Class 5),

- commencement of long-term monitoring of selected parameters (pH, Eh, Cl, SO₄ etc) at specific locations,
- (during the later CSI stage there is the possibility of supplementary Class 5 data from isolated sampling points in core-drilled boreholes in the upper bedrock).

3.3.3 Sub-surface information (> 100 m)

Some of this information will result from the ISI stage but mostly from the CSI stage characterised by deep drilling. This will include up to 10–20 core-drilled boreholes to around 700 m depth and an additional 5–10 percussion drillholes to 150–200 m. The ISI stage campaign will include 1–2 near-vertical core-drilled boreholes to around 1000 m or more and prioritised for hydrogeochemical studies. Groundwater sampling and analysis will be carried out during drilling of the cored boreholes (i.e. to obtain first indications of the ‘undisturbed’ groundwater environment) and subsequently from open boreholes and predetermined isolated borehole sections in the percussion and core-drilled boreholes. Emphasis in sampling, of course, will not be restricted to these cored boreholes which serve a special purpose; all borehole types will be sampled ensuring a wide spatial distribution of hydrogeochemical data for modelling purposes.

These sub-surface data will have a major impact on repository performance assessment and safety analysis since they will include characterisation of the ‘undisturbed’ groundwater environment at repository depths.

Output data covers sampling and analysis of:

- cored-drilled boreholes during drilling when a suitable fracture (zone) is intercepted or, failing that, at every approx. 100 m (Class 3),
- early logging/sampling (50 m sections) of additional percussion and core-drilled boreholes (Class 3),
- subsequent hydrochemical logging of these same additional percussion and core-drilled boreholes to determine borehole circulation trends (Class 3),
- 1–2 deep prioritised cored boreholes for hydrogeochemical characterisation at predetermined isolated borehole sections ($K = 10^{-6}$ – 10^{-8} ms⁻¹) (Class 5),
- additional cored boreholes for hydrogeochemical characterisation at predetermined isolated borehole sections ($K = 10^{-6}$ – 10^{-8} ms⁻¹) (Class 5),
- long-term monitoring (twice yearly) from at least 2 borehole sections selected from each borehole,
- fracture mineral characterisation from cored boreholes, in particular the 1–2 prioritised hydrogeochemical boreholes.

4 Management of uncertainties – general considerations

At every phase of the hydrogeochemical investigation programme – drilling, sampling, analysis, evaluation, modelling – uncertainties are introduced which have to be accounted for, addressed fully and clearly documented to provide confidence in the end result, whether it will be the site descriptive model or repository safety analysis and design. Handling the uncertainties involved in constructing a site descriptive model has been documented in detail by /Andersson, 2002/. These are summarised and listed below together with the areas of uncertainty of particular relevance (in italics) to the construction of a hydrogeochemical site descriptive model.

- **conceptual uncertainty** (i.e. a lack of understanding of processes and their interrelationships). This can also include the use of available models which are unsuitable, or that the model/modeller fails to describe the important processes or relationships. This may result in uncertainties which are so large that the link with reality becomes blurred or even lost altogether.

The uncertainties surrounding the construction of a site descriptive hydrogeochemical model are particularly complex since the model is partly based on several sub-modelling exercises and also has to interface with the other site descriptive models, in particular those covering geology and hydrogeology. There are three planned sub-modelling hydrogeochemical exercises:

- *traditional hydrogeochemical evaluation,*
- *principal component analysis (M3),*
- *geochemical equilibrium modelling (PHREEQC).*

To have confidence in the Hydrogeochemical Site Descriptive Model the uncertainties inherent in these three modelling components have to be addressed. In addition, /Andersson, 2002/ recommends not just a qualitative integration of hydrogeochemistry and hydrogeology to understand and describe the present groundwater conditions, but to further develop the possibility of using transient analysis in groundwater modelling whereupon the influence of, for example, isostatic recovery from the last glaciation, can be accommodated.

- **data uncertainty** (use of suspect parameter values in model construction, e.g. related to an error in the measurement, interpretation, extrapolation and interpolation of data, or based on an erroneous conceptualisation of important processes).

This is an important area in the hydrogeochemical investigations; examples include environmental contamination of the groundwater (e.g. agricultural pesticides and fertilisers etc), sampling/monitoring problems (e.g. erroneous pH and Eh values), analytical difficulties (e.g. Al) and insufficient data (e.g. leading to erroneous vertical and lateral extrapolation/interpolation).

- **spatial variability of data** (i.e. many properties vary considerably in space and this variability requires to be specified in the description). Several questions need to be posed: What spatial variability is there? What kind of description is needed? Is the variability smooth or irregular? The types of variability that require to be specified usually are problem dependent, for example sometimes a good average value suffices, sometimes a statistical description ('frequency' and 'amplitude') of the variation is what matters, and sometimes a very detailed description is required.

Confidence in the hydrogeochemical spatial variation of the chosen parameter values is considered to be essential when describing, for example, the radionuclide sorption properties (e.g. K_d) of the groundwater system.

- **chosen scale** (i.e. detailed or general description of spatial resolution over a specified minimum domain). Problems can arise if the wrong model boundary conditions are chosen or if there are inadequate data available to interpret too small or too large an area. A related issue is whether the scale of measurements is adequate for the desired scale of prediction. Furthermore, irrespective of the scale chosen there will be variability on a micro- or macro-scale, and this variability may be time-dependent.

From a hydrogeochemical perspective the scale of the deposition hole for the spent fuel container (i.e. repository near-field) is of major importance since it entails characterising the groundwater chemistry in the network of low transmissive micro-fractures/fissures in the rock matrix and predicting if and when such groundwaters will enter the deposition hole and interact with the engineered barrier system.

- **degree of confidence** (i.e. acceptance of a selected model description and its associated uncertainties as being correct in terms of understanding). Confidence mainly is a reflection of the availability of suitable data; the more data available, the greater the degree of confidence.

From a hydrogeochemical viewpoint, the more measured reliable data available, the better characterised/modelled is the represented volume, and the greater the confidence in its eventual use (e.g. in scenario development).

To further elaborate, the amount of data required for a certain confidence level depends on the complexity of the site, i.e. with little variation in the data, confidence in describing and understanding the history of a uncomplicated site is high even based on relatively few measurements. Contrastingly, a site characterised by a complex mixture of groundwaters, associated with uncertainties related to the choice of end members, equilibrium vs kinetic modelling, redox values, questionable palaeo-interpretation etc, the level of confidence will be low even though many measured data might be available. Assessing confidence, therefore, is not just a matter of accumulating data points.

In conclusion, the degree of confidence in a site description will depend not only on the amount and spatial distribution of the measured data that are available, but also on the complexity of the site. This leads on to another question: When are there enough data? This can only be resolved by asking what is the acceptable degree of uncertainty from a repository performance and safety assessment perspective.

- **risk analysis factor** (i.e. combination of the likelihood and consequences (usually dose) of a possible event(s) occurring in a geological repository).

Not readily seen as being relevant to the hydrogeochemical investigations.

- **error, precision, accuracy and bias** in forward predictions, either from measurements or models.

Since an important objective of the hydrogeochemical programme is to predict groundwater stability over repository timescales and the potential long-term impact on the integrity of the engineered barrier system, to quantify this area of uncertainty is highly relevant.

In conclusion, with the possible exception of the risk analysis factor (although /Andersson, 2002/ does point out that a safety analysis can be carried out using site descriptive models) all the above points have a direct relevance to the construction of a site descriptive hydrogeochemical model. When possible, these uncertainties are addressed systematically in Chapter 5 at each step of the hydrogeochemical evaluation/interpretation process.

5 Interpretation methodology

5.1 Stages involved

The various stages involved in the evaluation and interpretation of the hydrogeochemical data, and the interrelationships between the different stages shown earlier in Figure 1-1, are outlined again below in Figure 5-1 for convenience. The sequence illustrated can be applied at different junctures of the site investigations, for example, initially during the ISI investigation stage (e.g. version 1 as illustrated in Figure 5.1) and later during the CSI investigation stage (version 2) when additional and more comprehensive data become available. Once again, depending on the complexity of the site, additional iterations may have to be considered. These evaluations will result in a series of Hydrogeochemical Site Descriptive Models (e.g. Model versions x.x in Figure 5.1), each version representing the input of additional and new data with a corresponding updating and modification of the previous model. These iterations will lead eventually to a more complete Hydrogeochemical Site Descriptive Model. Based on this model, sub-models describing the surface, near-surface and sub-surface hydrogeochemical environments also may be constructed. The number, type and complexity of the sub-models will be determined when the nature of the site conditions become more apparent during the site investigations.

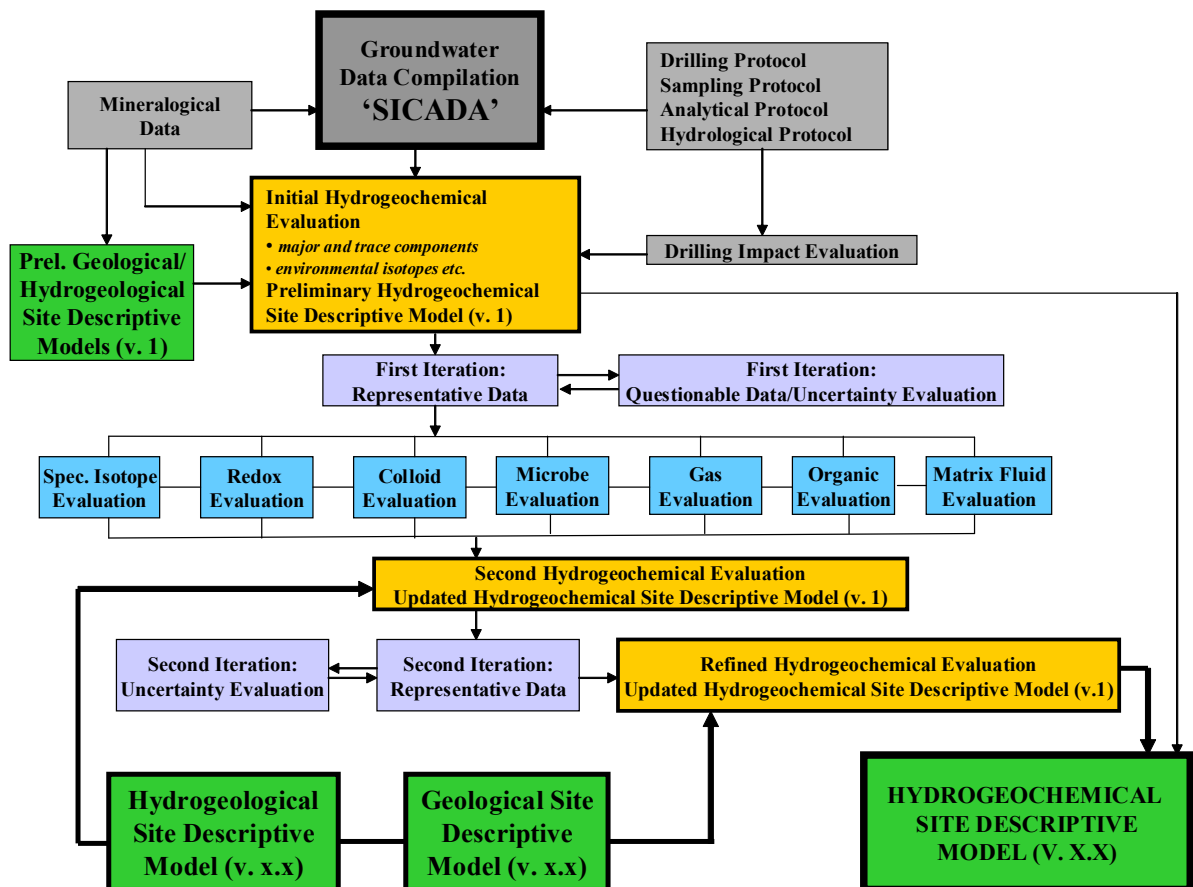


Figure 5-1. Flowchart showing the step-wise approach of integration and development involved in the hydrogeochemical evaluation of the Initial Site Investigation (ISI) stage to produce a site descriptive hydrogeochemical model. Yellow font indicates the major stages in the evaluation.

Figure 5-2 shows the extension of Figure 5-1 illustrating the important model decision-making stages prior to accepting a more complete Hydrogeochemical Site Descriptive Model (version x.x) and its subsequent use in safety and performance assessment.

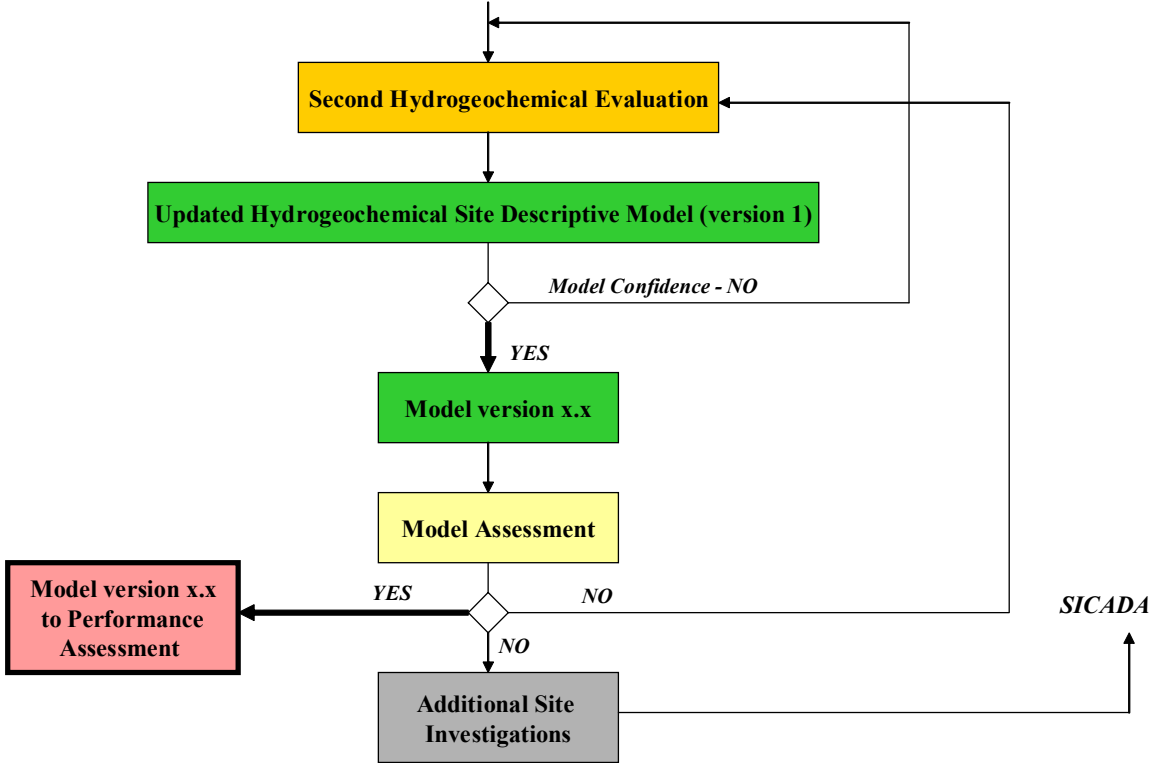


Figure 5-2. Flowchart showing the extension of Figure 5-1 illustrating the important stages of decision prior to continuing to a more complete Hydrogeochemical Site Descriptive Model (version x.x) and its subsequent use in Performance Assessment. If the initial or subsequent assessment of Model version x.x is negative, there is a loop back to the second hydrogeochemical evaluation stage, where additional data may be available, or a return to the site to collect new or complementary data. These new data will feed into the SKB geoscientific database SICADA.

Since an evaluation of the long-term radiological safety for the repository design proposed for the site is a major outcome of the site investigation phase, the decision-making stages indicated in Figure 5-2 are important. Establishing the reliability/confidence of the Hydrogeochemical Site Descriptive Models is intensified as the CSI stage nears completion. This includes the analysis of uncertainties and the development of alternative model concepts which lead to an evaluation as to whether the current site hydrogeochemical conditions and assumed transport properties can be explained by the spatial distribution of groundwater composition and the hydrodynamic flow situation. Consequently, certain model alternatives may be discarded and new ones created until one may prove to be more reasonable than the others although, in turn, this will also be subject to further examination including, for example, variation analyses to test its sensitivity /SKB, 2000/.

To best exemplify the hydrogeochemical evaluation strategy detailed below and outlined in Figure 5-1, the available data are assumed to result from the ISI stage. This will result in a preliminary hydrogeochemical site descriptive model version 1 resulting from the 'Initial Hydrogeochemical Evaluation' stage and an updated version 1 following the 'Second Hydrogeochemical Evaluation' stage. The Model version x.x indicated in Figure 5-1 should therefore represent the most complete model version resulting from the ISI stage (as addressed below), or subsequently resulting from the CSI stage.

5.2 Interpretation approach

Figure 5-1 identifies the overall data input source (i.e. SKB geoscientific database SICADA; /SKB, 2000/), the specific data input to each stage of the hydrogeochemical interpretation, and the main data output or result from each stage. Outlined below is a description of what is involved to complete each stage.

5.2.1 SICADA database

The SKB geoscientific database SICADA constitutes the major data source to the hydrogeochemical interpretation. In addition to a compilation of groundwater analytical data, SICADA contains:

- 'Associated Data/Information (i.e. Daily Logs)' of all field/site activities,
- various 'Protocols' relating to drilling, sampling, analysis and hydraulic measurements,
- mineralogical information.

Based on this background information, the groundwater chemical data contained in SICADA will have undergone an initial process of quality filtering. This considers discarding samples, for example:

- that have undergone excessive contamination (e.g. during drilling; short-circuiting around packer systems during monitoring/sampling etc),
- that have been subject to equipment failure (e.g. pump malfunction; packer maladjustment; malfunctioning electrodes etc),
- that have been subject to analytical inconsistencies in the laboratory (e.g. charge balance errors > 5%).

5.2.2 Initial hydrogeochemical evaluation

The first major assessment stage is the 'Initial Hydrogeochemical Evaluation', detailed in Figure 5-3. The available data at this stage will vary according to the progress of the site investigations and the timing of the evaluation. For example, during the early period of the ISI stage the data available will be those collected prior to the drilling of the first deep borehole and therefore will be restricted mostly to the surface and near-surface environments (~ 100 m). During the latter part of the ISI stage and the CSI stages, data input to the 'Initial Hydrogeochemical Evaluation' stage will be much more comprehensive since it will include a thorough study of the sub-surface bedrock environment (> 100 m).

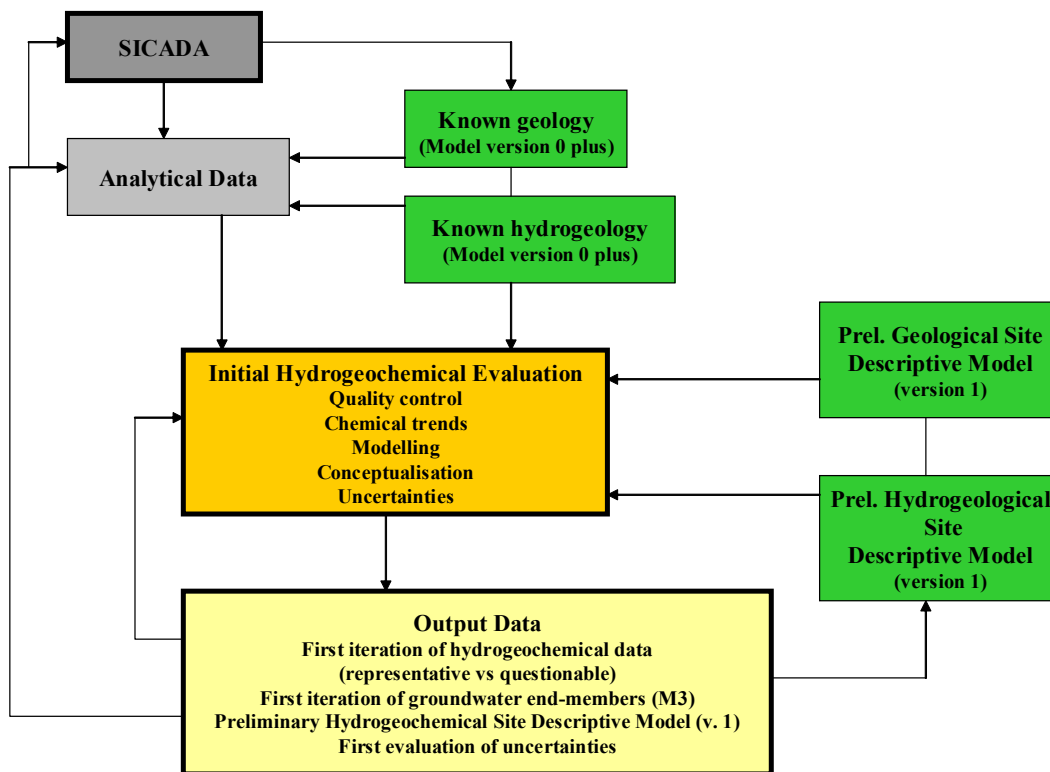


Figure 5-3. Flowchart showing details of the 'Initial Hydrogeochemical Evaluation' stage (see Figure 5-1).

Figure 5-3 shows the initial input to this evaluation stage comprises hydrogeochemical analytical data from SICADA plus the known geology and hydrogeology (model versions 0 plus). As investigations progress, updated geological and hydrogeological information will be continuously integrated (model versions 1), culminating eventually to produce a preliminary Hydrogeochemical Site Descriptive Model (version 1).

Input data

Analytical data

Early available input hydrogeochemical data resulting from the FS stage and ISI stage will include:

- major ions and most minor element constituents,
- field measurements of temperature (T), electrical conductivity (EC), dissolved oxygen (O₂), redox potential (Eh) and pH,
- environmental isotopes (³H, ²H, ¹⁸O, ¹³C and ¹⁴C).

Supporting geoscientific data

Hydrogeochemical interpretation is closely integrated with geology and hydrology. Input data requirements include (Figure 5-3):

- known geology (lithological and structural details; major fracture mineral phases etc),
- known hydrogeology (groundwater flow paths and directions; borehole hydraulics; water budgets at sampled borehole sections etc).

Evaluation of data

Evaluation of hydrogeochemical data falls under several main headings (Figure 5-3):

- quality control,
- chemical trends,
- modelling,
- conceptualisation,
- visualisation,
- uncertainties.

Quality control

General: Quality control in this context means a thorough assessment of all procedures involved in the location, sampling and analysis of groundwater samples that might give rise to inaccuracies or inconsistencies in the final groundwater chemical data. This will result in a breakdown of hydrogeochemical data into representative vs questionable/uncertain. 'Representative' can be strictly defined as a groundwater sample that accurately reflects the chemical (and hydraulic) conditions at the sampling location. Since in practice this is rarely achieved in a fractured crystalline bedrock environment due to influences from a host of activities (see below), a more realistic definition would be along the lines of 'A groundwater sample that closely reflects the chemical (and hydraulic) conditions at the sampling location' On this basis note that 'Questionable or uncertain data' does not refer to data which should be removed totally from the dataset, although this may be warranted in some extreme cases that bypass the SICADA filtering process (see section 5.1.1). Questionable or uncertain data may be representative from a major ion viewpoint, yet not representative, for example, from a more sensitive redox or colloid viewpoint. Such data still may therefore be used under certain circumstances (e.g. modelling large-scale groundwater trends), but their use in other areas (e.g. geochemical equilibrium modelling) may have to be limited, or excluded, as the case may be.

Some analyses deemed unsuitable may prove eventually to be useful by considering at an early stage the uncertainties giving rise to the unsuitability. For example, in practice a 'Hydrogeochemical Analysis Group' (HAG), responsible to the overall SKB Site Analysis Team, has been formed to actively oversee and advise the on-going hydrogeochemical site programme. In part this will entail checking the drilling and borehole activity protocols to gain an understanding as to which samples may or may not be suitable. Based on this early stage evaluation, the Group will be in the position to recommend additional sampling or modifications to sampling locations and procedures.

The first step of the initial hydrogeochemical evaluation stage will function basically as a recheck on the quality of the SICADA database and also provide a first iteration of representative vs questionable/uncertain data. The approach to groundwater quality control, based on previous site investigation experience in Sweden, is detailed in /Smellie et al, 1985/, /Smellie and Laaksoharju, 1992/, /Laaksoharju et al, 1993/ and /Smellie et al, 1999/. The impact of drilling is described in /Gurban and Laaksoharju, 2002/ and the analytical data compiled in the SICADA database is subject to a strict laboratory quality control.

Previous experience shows that the assessment of groundwater quality (representative vs questionable data) requires detailed knowledge of potential sources of error. For example, major sources of groundwater contamination derive from borehole activities such as:

- drilling and borehole cleaning,
- open borehole effects,
- downhole geophysical/geochemical logging,
- downhole hydraulic logging/testing/pumping,
- downhole sampling of groundwaters.

Additional sources of error/uncertainty derive from sampling and analytical procedures:

- sample handling, transportation and preparation,
- analytical error associated with downhole measurements of pH and Eh (e.g. Chemmac),
- analytical error associated with laboratory measurements (major and trace elements, isotopes, gases etc).

Uncertainty evaluation: As discussed under Chapter 4, there is a requirement to quantify the uncertainties surrounding some of the groundwater input data and the consequences of using such data in assessing groundwater quality and ultimately their use in model construction. Some of the uncertainties, however, are difficult to describe; for example, since there are no ‘undisturbed’ samples to provide a reference point, uncertainties associated with groundwater sampling will be difficult to resolve. This dilemma can be partly compensated for by controlling (and modelling) those major disturbing influences on groundwater quality.

For example:

- measure/model the input and output water volumes along different fractures/fracture zones in association with drilling and other borehole activities (i.e. DIS: Drilling Impact Study). This approach, combined with measured borehole hydraulic parameters (i.e. conductivity and piezometric head) will essentially produce the total water budget for each sampled section thus facilitating the selection of groundwater samples judged to be more representative,
- measure the chemical variation during sampling which can indicate the ‘natural’ variability,
- measure the direct influence of the spiked flushing water resulting from drilling,
- measure/model the effect of transporting water from depth to the surface (e.g. to quantify the influence of in- and out-gassing processes on redox measurements).

Nevertheless, issues which can be measured/modelled subsequently may be used in models to test their influence on the results. Such modelling, by necessity, will be site or borehole specific since there is no 'undisturbed' groundwater reference point to provide a precise measure of uncertainty. At best only estimates of the most important uncertainties are presently possible.

Other issues of importance concern laboratory sample preparation and analysis. In contrast to the quality of groundwater sampling, which is generally unpredictable and borehole/fracture specific, sample preparation procedures and analytical precision are predictable and the uncertainties are easily evaluated.

From field, *in-situ* and laboratory measurements, the following examples of estimated uncertainties are based on field evidence and modelling from the Äspö site investigations:

- drilling; may be $\pm 10\text{--}20\%$ of the measured or calculated value from water budget calculations,
- sampling; may be $\pm 10\%$ of the measured or calculated value from time-series variations of major ions during pumping,
- influence (e.g. on Eh) associated with the uplifting and sampling of water from depth to surface; may be $\pm 10\%$ of the measured or calculated value based on modelling,
- sample handling and preparation; may be $\pm 5\%$ of the measured or calculated value based on modelling the influence of atmospheric gases,
- analytical error associated with laboratory measurements; is $\pm 5\%$ of the measured value for the major components.

Chemical and isotopic trends

General: Based on a reliable database, the next stage is to establish any significant groundwater chemical and isotopic trends which may be related to one or more of the following:

- depth variations,
- lateral variations,
- time-series variations during sampling (i.e. continuous; sporadic),
- time-series variations between sampling occasions,
- evidence of rock/water reactions (e.g. dissolution/precipitation; ion-exchange etc),
- evidence of other reactions (e.g. microbially-mediated),
- evidence of palaeohydrogeochemical trends (e.g. signatures of past glacial events),
- identification and mixing of different groundwater end-members.

The recognition of such trends and their relationship to groundwater mixing and geochemical evolution processes can be greatly aided by available computer software. In this respect it is planned to use: 1) AquaChem (Aqueous geochemical data analysis, plotting and modelling tool; Waterloo Hydrogeologic, 2) ChemStat (Advanced chemical statistical program; The Scientific Software Group), and 3) TECPLOT (2D/3D interpolation, visualisation and animation tool; Amtec Engineering Ltd).

Uncertainty evaluation: The uncertainties associated in interpreting chemical and isotopic trends are dependent on the input data (addressed above under ‘Quality control’) and also on the nature of the computer software used in classifying, evaluating and modelling the data. In general, most software packages have no fixed uncertainties; the main uncertainties relate to the simplifications and assumptions written into the codes. To evaluate the uncertainties involved in treating the groundwater data is therefore a complex issue and this is made even more complicated by additional uncertainties reflecting the nature of the data which are generally site-specific and involve criteria such as quality, distribution and variation. Uncertainties can be tested by using given data, alternative models or comparison with independent models or modelling approaches. When using simple interpolation approaches such as scatter plots the uncertainty is dependent on data quality; when using complex 3D interpolation, distribution of data determines the main uncertainties.

Attempts should be made to illustrate the uncertainties associated with the various interpolations by producing a series of site visualisations testing different ideas and assumptions. For example, at sites characterised by a concentration of measured points associated with one or two boreholes (e.g. Laxemar) or a group of boreholes surrounded by sporadically distributed measured points from outlying borehole locations, there is a danger that the latter (i.e. little known boundary conditions) may unduly control too much of the resulting distribution. It might be better to show the interpolation within a justifiable ‘radius of influence’ (e.g. with adequate data points) and leave the rest of the domain ‘grey’; this could be illustrated by grading (using colour for example) the varying degrees of confidence in the modelled site area.

Hydrogeochemical modelling

General: To further confirm and quantify some of the chemical processes and mechanisms indicated under ‘Chemical and isotopic trends’, two specific hydrogeochemical modelling approaches will be employed to address:

- rock/water reactions (e.g. dissolution/precipitation; ion-exchange etc),
- mixing of different groundwater end-members.

To cover rock/water reactions the PHREEQC (Version 2) code, developed by the USGS (Boulder, Colorado, USA), will be used, and to cover end-member mixing processes (including palaeo-trends) and an overall statistical appraisal of the hydrochemical data, the Multivariate Mixing and Mass Balance Calculations (Version 2) program, developed by /Laaksoharju et al, 1999a/, will be used.

Use of these modelling approaches will also lend further support to the presence or absence of microbially-mediated reactions and provide additional insight into the palaeo-evolution of the groundwater system.

Uncertainty evaluation: Hydrogeochemical modelling also introduces uncertainties which vary in complexity. The uncertainties involved in the Multivariate Mixing and Mass Balance (M3) calculations have been identified and addressed by /Laaksoharju, 1999/ and /Laaksoharju et al, 1999b/. The M3 uncertainties for the mixing calculations applied to the Äspö data are of the order of $\pm 10\%$ within a 95% confidence interval. The major uncertainties are due to assumptions and simplifications used in the model.

Uncertainties inherent in the PHREEQC (Version 2) program also have been addressed /e.g. Parkhurst et al, 1980; Alley, 1993; Laaksoharju, 1999/. These depend on which model is used in PHREEQC. Generally the analytical uncertainties (e.g. Al determinations) and uncertainties concerning the thermodynamic databases are of importance. For example, one unit error in the pH measurements results in one unit error in the saturation index calculations which can lead to misunderstandings concerning the under-/super-saturation of the groundwater in respect to various minerals. Care also is required to select mineral phases which are realistic (even better if they have been positively identified and analysed) for the systems being modelled.

When using modelling options available in PHREEQC, for example, the inverse modelling approach, the assumptions made by the modeller determine the uncertainties. The site specific uncertainties for the models described above can be tested by using quantified uncertainties, alternative models and comparisons with independent models.

Conceptualisation/Visualisation

General: Based on the evaluation of chemical and isotopic trends and subsequent hydrogeochemical modelling, a preliminary hydrogeochemical descriptive model on a site scale will be produced illustrating, for example:

- presence and location of major groundwater bodies,
- depth variations (e.g. major and trace element chemistry; redox) within each groundwater body,
- lateral variations (e.g. major and trace element chemistry; redox) within each groundwater body,
- areas influenced/dominated by water/rock reactions,
- areas influenced/dominated by microbially-mediated reactions,
- areas influenced/dominated by mixing,
- integration with latest geological and hydrogeological interpretations,
- indication of major groundwater flow directions.

The detail of conceptualisation and the nature of the visualisation (i.e. 2D/3D interpolation and fracture media visualisation) will depend largely on the nature and detail of the available geological and hydrogeological information. In practice, when more data are available, several modelling approaches will probably be integrated to provide a best representation of the site.

Uncertainty evaluation: For the TECPLOT interpolations the uncertainties are site and data specific where the distribution of data plays a major role together with the assumptions made concerning the boundary conditions. The site specific uncertainties can be tested by using quantified uncertainties, alternative models, and comparison with independent models.

Since hydrogeochemical conceptualisation incorporates geological and hydrological information, introduced uncertainties from these two disciplines need also to be evaluated.

Output data

The major output data from the 'Initial Hydrogeochemical Evaluation' stage (Figure 5-3) will be:

- a first iteration of hydrogeochemical data into representative/questionable,
- a first iteration of groundwater end-members and degree of mixing using M3,
- a first iteration of rock/water reactions using PHREEQC,
- a preliminary Hydrogeochemical Site Descriptive Model (version 1),
- a preliminary description of palaeohydrogeochemical events,
- a first evaluation of uncertainties.

5.2.3 Evaluation of specialised study areas

In parallel with the initial hydrogeochemical evaluation stage new, limited, but more specific analytical data will become available. These data, mostly from sampling the 1–2 prioritised hydrogeochemical boreholes (i.e. ISI Stage), provide the basis for the evaluation of several areas of specialised study covering isotope systematics, redox chemistry and dissolved gases, and the characterisation of colloids, microbes and organics, present in the groundwaters, together with the characterisation of the interconnected pore space fluids/groundwaters in the rock matrix (Figure 5-1). Evaluation within these areas will be based therefore on output from the initial hydrogeochemical evaluation stage together with additional input data specific to each area of specialised study.

There is an obvious yet unavoidable degree of overlap with the specialised isotope and redox evaluations and use of similar data in the initial hydrogeochemical evaluation stage. However the isotope overlap will be limited to the environmental isotopes (^3H , ^2H , ^{18}O , ^{13}C and ^{14}C), thus emphasising the more exotic isotopes (^{34}S , ^{87}Sr , ^{86}Sr , ^3He , ^4He , ^{37}Cl , ^{11}B , ^{36}Cl , $^{234}\text{U}/^{238}\text{U}$, ^{226}Ra , Rn) for the specialised evaluation stage. For the redox evaluation the overlap will be limited to field Eh measurements and Fe(II) and Fe(III) analyses.

In addition to providing a detailed evaluation and interpretation of the specialised data, which may be seen as topic-specific and not readily of direct use, these data fulfil several very important functions. For example, they provide a further test on the suitability/unsuitability of the chemical data, provide support or otherwise on the choice of groundwater end-members used in the M3 calculations and, perhaps most importantly, they provide input data to safety and performance assessments (e.g. redox conditions and spent fuel stability; the potential influence of colloids/organics/microbes on radionuclide transport; bedrock groundwater residence times etc).

Note that since these specialised study areas are mainly restricted to selected, high quality groundwater/gas samples from the 1–2 prioritised hydrogeochemical boreholes, their wider use in constructing the hydrogeochemical site description model will be limited.

Determining the matrix or interconnected pore space fluid/water in representative low permeable bedrock types could provide an important end-member for hydrogeochemical modelling purposes in addition to valuable chemical input data to near-field repository safety and performance calculations.

Specialised isotope evaluation

This evaluation provides important support and confirmation of present-day groundwater evolution and mixing processes. Equally important, their value in tracing palaeohydrogeochemical events is critical in understanding the long-term evolution of the site.

Input data

The input data will constitute isotope analyses of groundwater (including low transmissive rock matrix fluids/groundwaters) and gas samples selected from the SICADA database. The data will be divided into three groups:

- Stable isotope ratios (in addition to $\delta^{18}\text{O}$ and $\delta^2\text{H}$): $\delta^{13}\text{C}$, $\delta^{34}\text{S}$, $\delta^{37}\text{Cl}$, and $\delta^{11}\text{B}$.
- Radiogenic stable isotopes: $\delta^{87}\text{Sr}$, $^4\text{He}/^3\text{He}$.
- Radioactive isotopes: ^{36}Cl , ^3H , ^{14}C , Uranium-series isotopes ($^{234}\text{U}/^{238}\text{U}$, ^{226}Ra , Rn).

There will probably not be a complete set of data including all the above-mentioned isotopes from all of the sampled localities. This will reflect, for example, the low carbonate content in very saline groundwaters (if present) making carbon isotope analyses impossible etc.

Data from isotope analyses of fracture fillings and altered adjacent wall rock, particularly when in contact with the sampled groundwaters, will also be used in the interpretation of the groundwater data.

Evaluation of data

Data evaluation will focus on the following areas of interest:

- depth variations,
- lateral variations,
- estimates of residence times of the groundwater or components in the water,
- time-series variations between sampling occasions; for example successive sampling of cosmogenic isotopes like ^{36}Cl , ^3H , ^{14}C showing variations (decrease/increase) of recent groundwater components,
- evidence of rock/water reactions; for example ion exchange and silicate weathering can be studied using $\delta^{87}\text{Sr}$; calcite/groundwater interaction will be studied using $\delta^{13}\text{C}$ and $\delta^{18}\text{O}$; removal and deposition of U will be studied using U-series data from groundwater and fracture filling materials,
- evidence of microbially-mediated reactions; especially $\delta^{13}\text{C}$ and $\delta^{34}\text{S}$ can help to trace microbial activity in the fracture minerals as well as in groundwaters,
- evidence of palaeohydrogeochemical trends (e.g. signatures of past glacial events); interpretations of palaeohydrogeological regimes based on data (e.g. $\delta^{18}\text{O}$, $\delta^2\text{H}$ and ^{14}C) from fracture minerals (mainly calcites),
- identification of groundwater end-members using all the available information on the end-member samples; the isotope data can help in revealing the processes that have affected the end-members and will give a time frame for the residence of that groundwater (or components in the water, e.g. using Cl and HCO_3),

- uranium isotopes (used for studies of uranium mobilisation/deposition) and $\delta^{13}\text{C}$ and $\delta^{34}\text{S}$ (used for interpretation of biogenic activity) may also provide support for the evaluation of redox conditions described below.

Uncertainty evaluation: ‘Age dating’ of groundwater is almost an impossible task and instead the term ‘Mean residence time’ is frequently used, which is still somewhat misleading. For example, using ^{36}Cl only dates the chlorine component and not the water *sensu stricto*, thus complex groundwater mixing processes involving chloride-rich waters of different origins and ages may create a ‘mean residence time’ which is meaningless.

Interpretations of calcite/groundwater equilibria using $\delta^{18}\text{O}$ data require information of the formation temperature in order to calculate the $\delta^{18}\text{O}$ for the water (if the $\delta^{18}\text{O}$ of the calcite is known and vice versa). Very often temperature data are lacking and less precise temperature indicators often have to be used. For all types of mineral/water interaction modelling, the basic assumption is that the groundwater analysed has been in contact with the actual fracture mineral(s) analysed, thus the $\delta^{18}\text{O}$ data can be interpreted accordingly. In reality, however, this is very hard to prove and the degree of uncertainty will reflect the success or otherwise of the groundwater sampling procedures.

Output data

A major advantage of these isotopic data is their use to confirm/support/explain the earlier modelled distribution and interpretation of the major groundwater ions and trace elements on a much more sensitive and accurate basis, and also to shed some understanding on past events of climate change. The major output data from the isotope evaluation will be:

- to interpret the origin of the end-members revealed by the hydrogeochemical data modelling,
- to indicate rock/water interactions (e.g. to be compared with the PHREEQC modelling results),
- to interpret long-term hydrochemical stability over time using stable and radiogenic isotopes in groundwater, matrix pore space fluids/groundwaters and fracture minerals,
- to estimate groundwater residence times,
- to provide input to the hydrogeochemical site descriptive model.

Redox evaluation

Measurement and interpretation of groundwater redox conditions are critical to first evaluate the suitability of a site for hosting a repository, and then to predict the long-term stability and safety of the repository during its expected lifespan of thousands to hundreds of thousands of years.

An obvious approach is to measure the dissolved oxygen content in the groundwaters, both *in-situ* and analysis of headspace gas in the laboratory from collected samples. However, even if the groundwater contains no dissolved oxygen, measurement and analysis will never register zero and thus will be reported as less than the detection

limit. To overcome this uncertainty, other criteria will be used, for example initially the presence of Fe(II) or sulphide (S^-) in the groundwaters, and secondly the Eh (redox potential) of the groundwaters. However, because of the low solubility of iron sulphides it is not possible to detect both dissolved Fe(II) and sulphide.

Input data

The input data consist of:

- Eh (mV) from three electrodes (i.e. gold, platinum and graphite),
- groundwater concentrations of important redox-sensitive components (i.e. total Fe, Fe(II), Mn, sulphide, ammonium),
- groundwater concentrations of several trace elements (some redox-sensitive) such as Al, REEs, Mo, Ni etc.

Further input may result from the colloid, microbial and gas studies outlined below.

Evaluation of data

Data evaluation will focus on the following areas:

- artefact evaluation (i.e. estimate possible effects of contamination, mainly from atmospheric oxygen, but also from air-saturated drilling fluids),
- qualitative consistency between measured Eh values, and between the Eh data and the analysed iron, sulphur, manganese and nitrogen species.

The evaluation of redox conditions will also rely on other data such as colloids, microbes and gases.

Uncertainty evaluation: A proper assessment of redox groundwater conditions is strongly linked to the availability of field facilities for rapid chemical analysis (e.g. total Fe and Fe(II)) and down-hole measuring probes. Hydrological constraints might influence the possibility of atmospheric contamination, for example, low groundwater flow-rates give long residence times in the sampling tubes thus increasing the diffusion of atmospheric oxygen into the waters.

Output data

The main output from the redox evaluation of the groundwaters will be:

- confirmation of their reducing conditions,
- confirmation of their reducing capacity as a function of depth and horizontal coordinates,
- evidence of microbially-mediated sulphate reduction.

Colloid evaluation

Standard radionuclide transport models implicitly assume that radionuclides are only transported as dissolved species in the groundwater. This neglects, however, the potential effect of advective transport of radionuclides bound to colloid particles /McCarthy and Degueldre, 1991/. To address this issue, the collection, analysis and

interpretation of colloidal material will form an integral part of the hydrogeochemical site investigative programme.

Input data

Input data (including estimates of uncertainty) comprise:

- inorganic element content on filters/water (can be $\pm 10\%$),
- particle counting (can be $\pm 10\%$),
- organic material (can be $\pm 10\%$),
- microorganisms ($\pm 10\%$).

Evaluation of data

Quality control for colloidal data comprises the following set of tasks:

- Avoiding chemical changes due to uplifting of water, contamination from air or particles in air during analysis and sample handling /Laaksoharju et al, 1995/.
- Colloid samples should be collected using *in-situ* sample vessels to ensure pressurised samples; analyses such as particle counting should be performed under such maintained pressure conditions. Filtering should be performed on-line under a positive inert atmosphere.
- Artefact evaluation, where the possible effects from contamination are evaluated and modelled /Laaksoharju et al, 1995/.

The data obtained can be used for various modelling purposes:

- The number of colloids will determine the radionuclide transport properties of the groundwater and is an important safety variable.
- The type of colloid is of interest since, for example, silica colloids are more stable than calcite colloids and the former have therefore a higher potential as a radionuclide carrier. Microbes can respond to changes in the environment and can migrate.

Conceptualisation and visualisation can be performed in several ways (e.g. depth, 2D and 3D) in connection with other groundwater properties which affect the stability or chemical properties of colloids (e.g. salinity and redox conditions).

Uncertainty evaluation: A major area of uncertainty involves the sampling and handling procedures for colloids in the field; in common with the groundwater sampling procedures these uncertainties are kept as much as possible to a minimum. In the laboratory uncertainties (e.g. analytical) can be reasonably well estimated; these are given in parenthesis with the input data above.

Output data

The major output from the colloid evaluation is:

- to determine the number and type of colloids,
- to determine the stability of the various colloids under present and changing groundwater conditions.

The final product is to derive a concentration range of potentially stable colloids to be used as input to safety assessment modelling.

Microbe evaluation

Microbes in large numbers, 10^6 – 10^9 cells per L /Pedersen, 2001/, exist naturally in deep groundwaters and may have a significant effect on the groundwater chemistry /Stumm and Morgan, 1981/. During the construction and operational stages of a repository, large numbers and different species of microbes will be introduced to the groundwater and repository environments, but some species may not be viable following repository closure. However, sufficiently large microbial populations may survive in the groundwater and repository environment to have an effect on the geochemistry of those environments although their potential efficiency very much depends on the supply of nutrients and the degree of extreme conditions such as high temperature, high pH, desiccation and radiation effects. The repercussions of microbial activity on high-level repository performance include gas generation, canister corrosion, redox reactions, formation of complexing agents and groundwater radionuclide transport. The extent to which they will be able to colonise the near-field and far-field repository environments therefore is an important issue to address in long-term repository safety and performance assessment.

Input data

Input data (including estimates of uncertainty) comprise the:

- total number of microorganisms ($\pm 10\%$),
- quantity and activity of sulphate reducing bacteria ($\pm 20\%$),
- quantity and activity of autotrophic and heterotrophic methanogens ($\pm 20\%$),
- quantity and activity of autotrophic and heterotrophic acetogens ($\pm 20\%$),
- quantity and activity of oxygen reducing microorganisms ($\pm 20\%$).

Evaluation of data

The quality control for microbial data comprises the following set of tasks:

- Drilling operations may introduce microbes from the surface environment and the drilling rig itself (tubings, tanks etc) into the aquifers /Pedersen et al, 1997/. Therefore, it is required that drilling fluids are kept sterile using ultra-violet light sterilisation procedures. All drilling equipment should also be sterilised by suitable methods (e.g. steam cleaning, washing with bleach or alcohol). Control samples of the drilling waters are required using experimental protocols identical to the ones applied to the borehole samples.
- Control water samples should be obtained at the surface using the sample vessel and equipment for borehole sampling. Sampling of sterile waters will provide negative controls and will be important in the evaluation of achieved equipment hygiene /Haveman et al, 1999/.

The data obtained can be used for various modelling purposes:

- The total numbers of microorganisms are valuable for colloid modelling because microbes, just as colloids, may act as sorbents and provide transport mechanisms in the event of radionuclide release from the near-field..
- The quantities of different physiological groups of microorganisms are needed to support the microbial activity measurements, for example, using radioisotope techniques as described in /Pedersen, 2001/. A measured sulphate reduction should preferably be supported by observations of the presence of sulphate-reducing bacteria.
- The presence or absence of on-going microbially mediated reactions will be inferred by activity data.

Conceptualisation and visualisation of microbial activity can be performed in several different ways. Depth variation can be carried out for all parameters measured. Significant correlations between microbial data and geological or hydrogeochemical data are, at present, rarely attempted and, if done, are not always successful. Therefore, data from all related disciplines must be treated and analysed together. This may be accomplished by superimposing numbers of organisms and activities in M3 plots and mixing calculations. This will give information on the relation between different types of mixing groundwaters and microbial activity /Haveman and Pedersen, 2002/, and the influence of microbes on radionuclide transport may also be inferred. The detailed conceptualisation will depend largely on the outcome of the M3 modelling comparison.

Uncertainty evaluation: A major area of uncertainty involves the sampling and handling procedures in the field; in common with the groundwater sampling procedures these uncertainties are kept as much as possible to a minimum. In the laboratory uncertainties (e.g. analytical) can be reasonably well estimated; these are given in parenthesis with the input data above.

The degree of uncertainty depends partly on the final choice of methods. Molecular biology methods cover a large proportion of the populations present, but the error can sometimes be large due to bias in the gene amplification steps. Culturing methods have a very good precision but typically only pick up 0.2 % (average) of the total number of cells present. *In-situ* activity methods are generally satisfactory with respect to population coverage but as the populations will become disturbed during sampling an uncertainty appears that is difficult to evaluate. *In-situ* molecular methods give a better prediction of the *in-situ* conditions, but possible bias in gene amplification must be carefully controlled. A combination of culturing and molecular biology methods, possibly including Phospholipid Fatty Acid (PLFA) analysis, will give the most complete and accurate picture of what organisms are present.

Output data

The major output data from microbial evaluation will be information concerning those bedrock/fracture areas influenced or dominated by microbially mediated reactions. Of particular importance will be microbially mediated redox controls, sulphate reduction and carbon cycling.

Gas evaluation

Gases may be generated under oxidising conditions in a repository shortly after closure, and may in the long-term be generated when conditions become dominantly chemically reducing. Natural accumulation of gases from depth will also occur (e.g. methane). Accumulation of gases may result in a gas over pressure which might cause physical damage to the engineered barriers. In a HLW repository the production of hydrogen gas from the anaerobic corrosion of the large amount of steel is the most important process; microbially induced anaerobic degradation of organic material and the radiolysis of water are considered of less importance.

Input data

Input data (including estimates of uncertainty) comprise:

- the total volume of dissolved gases in groundwater ($\pm 5\%$),
- the concentration of dissolved H_2 , He, Ar, N_2 , CO, CO_2 , CH_4 , C_2H_6 and C_2H_4 ($\pm 5\%$),
- the presence/absence of oxygen ($\pm 10\%$),
- the $^{13}C/^{12}C$ ratio of dissolved methane ($\pm 10\%$).

Evaluation of data

Quality control for gas comprises the following tasks:

- Measurement of standard mixtures of gases typically observed in groundwater; this will control the quality of the analytical procedures.
- The extraction of gas from the sample, this process is difficult and the potential for leakage of air into the analytical system is large. The presence of oxygen in a ferrous iron/sulphide containing water sample indicates such leakage. Oxygen can be used as a control parameter provided an alternative method is used to test for the absolute presence/absence of oxygen. Winkler titration or possibly optrodes (optical electrodes are soon to be on the market) can be used for this purpose.

The gas data will be used to model gas saturation. The $^{13}CH_4/^{12}CH_4$ ratio suggests the origin of the methane and should be treated together with microbial data. Gas data are best visualised in standard table and graph formats in relation to depth. Presence/absence of oxygen is of significant importance. The test hypothesis will be that oxygen is absent in the presence of dissolved ferrous iron and/or sulphide. The CO_2 concentration should correlate with the carbonate concentrations if normalised to a specific chemical environment. It is possible that gas data and M3 modelling will show correlations, i.e. gas concentrations are related to various end members. This can easily be tested once results are available.

Uncertainty evaluation: A major area of uncertainty involves the sampling and handling procedures in the field; in common with the groundwater sampling procedures these uncertainties are kept as much as possible to a minimum. In the laboratory uncertainties (e.g. analytical) can be reasonably well estimated; these are given in parenthesis with the input data above.

With respect to sampling and handling procedures in the field, from earlier experience leakage of air into the sample during processing is a significant uncertainty. This may typically occur during the transfer of the sample from the sampling vessel to the gas extractor and onwards to the gas chromatograph. This error results in exaggerated high values of nitrogen and oxygen. As groundwaters generally are anoxic, this error can be corrected by subtracting the oxygen content and 4 times the oxygen content of nitrogen from the obtained data.

Output data

The gas data will be presented in relation to saturation of each gas at ambient pressure and at atmospheric (tunnel) pressure; the absence/presence of oxygen will be discussed. The possible sources of the gases will be listed.

Organic carbon evaluation

The presence of natural organic compounds in groundwaters, notably humic substances and other organic chelators which can form strong complexes with highly charged ions (e.g. actinides), may influence the mobilisation and transport of radionuclides from the near-field to the far-field of a repository /Choppin and Allard, 1985/.

Input data

Input data (including estimates of uncertainty) comprise:

- the concentration of total organic carbon (TOC) ($\pm 10\%$),
- the concentration of dissolved organic carbon (DOC) ($\pm 10\%$),
- the proportion of acetate in DOC ($\pm 10\%$),
- the proportion of fulvic and humic acids in DOC ($\pm 10\%$).

Evaluation of data

The quality control for organic compounds comprises two tasks:

- Tubing and other material with organic matrices in contact with the groundwater and the sample will be tested for their potential to leak organic carbon of any kind. Exposing sterile, organic carbon-free distilled water to the equipment in use provides some degree of sample control.
- The quality and precision of the analytical procedures may be affected by groundwater and salinity. Interferences of this kind must be kept under control.

The amount of organic carbon is a potential source of energy for microbes, especially in the case of oxygen introduction into aquifers. This can be used in the modelling of redox conditions and redox buffer capacity of the groundwater. The concentration of organic carbon usually decreases with depth. Dissolved acetate is expected to originate from either microbial autotrophic CO₂ fixation processes, or from degradation of larger organic molecules. Fulvic and humic acids are expected to be resistant to microbial degradation.

Uncertainty evaluation: A major area of uncertainty involves the sampling and handling procedures in the field; in common with the groundwater sampling procedures these uncertainties are kept as much as possible to a minimum. In the laboratory uncertainties (e.g. analytical) can be reasonably well estimated; these are given in parenthesis with the input data above. Provided the quality control discussed above is accurately performed, uncertainties will typically be natural variation of samples and analytical errors. They can be dealt with by analysing independent samples.

Output data

The organic carbon data will be presented in table and graph formats.

Matrix fluid evaluation

To better understand the hydrogeochemical character of low permeable rock masses (i.e. those rock units demarcated for canister disposal of the radioactive wastes), laboratory-based diffusion experiments will be conducted on drillcore sections to determine the chemistry of the interconnected pore space fluids/groundwaters in the rock matrix /Smellie et al, 2000/.

Input data

Input data comprise:

- mineralogy of rock matrix drillcore sections (representing major lithologies; depth profiles; profiles from water-conducting fractures, or fracture zones, into the surrounding rock matrix),
- fluid inclusion characterisation (population types; volume and composition of fluids),
- composition of extracted gases from core samples in sealed containers (^4He , ^3He),
- composition of extracted matrix pore space fluid/water from diffusion experiments (major and trace element chemistry; $\delta^{18}\text{O}$, $\delta^2\text{H}$, $\delta^{13}\text{C}$, ^{14}C , $\delta^{37}\text{Cl}$, $\delta^{11}\text{B}$, $\delta^{87}\text{Sr}$).

Evaluation of data

Evaluation of the data will involve the following main issues:

- to locate, identify and characterise chemically the fluid inclusion populations in the rock matrix,
- to seek evidence if fluid inclusions may be contributing (by leakage or reaction) to the chemistry of the interconnected pore space fluids/groundwaters,
- to determine the interconnected pore space porosity,
- to model geochemically the expected matrix pore space fluid chemistry,
- to extract the interconnected pore space fluids and gases,
- to compare modelled pore space fluid/groundwater chemistry with the extracted fluid/groundwater composition resulting from the diffusion experiments.

Uncertainty evaluation: An obvious area of uncertainty involves sampling procedures in the field to ensure that fracture-free samples are selected and that lithological variations are accommodated. In any case the planned detailed microscopic studies should minimise such uncertainties by ultimately selecting the most suitable samples.

To avoid unnecessary evaporation of matrix pore space fluids/groundwaters following removal of the drillcore (i.e. a further area of potential uncertainty), rapid preservation of the sampled drillcores in the field will be necessary.

In the laboratory, analytical uncertainties can be reasonably well estimated. Furthermore, the optimum time for the diffusion studies to extract the interconnected pore space fluid/groundwater will be carefully monitored and adjusted during the experiment so that adequate time is available.

Interconnected porosity measurements may be influenced by stress-release processes acting on the drillcore lengths following drilling, removal and storage. Such influences are difficult to quantify although estimations are possible.

Provided the quality controls discussed above are rigorously performed, uncertainties will typically be natural variation of samples and laboratory analytical errors.

Output data

The main output data will provide:

- the chemistry of the interconnected pore space fluid/groundwater and associated gases (namely ^4He , ^3He).

Closely linked is:

- to show whether the extracted matrix or pore space fluid/groundwater corresponds to modelled expectations (i.e. presently in equilibrium with the rock matrix),
- to show whether the extracted matrix or pore space fluid/groundwater has alternative (external?) sources (i.e. presently at disequilibrium with the rock matrix),
- to show whether the extracted matrix or pore space fluid/groundwater and gases show any systematic variation in space (i.e. evidence of an in- or out-diffusion profile) towards a well established water-conducting fracture (or fracture zone). This should help characterise the dominant transport mechanism for individual solutes (diffusion vs advection) and, in the best case, to their individual *in-situ* diffusion constants.

5.2.4 Second hydrogeochemical evaluation

The second main evaluation in the hydrogeochemical site characterisation (Figure 5-1) will involve significant groundwater input data from depth (>100 m). Included will be data from the drilling and preliminary sampling of the 1–2 prioritised hydrogeochemical boreholes (i.e. latter part of the ISI Stage) and preliminary results from the specialised areas of study (i.e. special isotopes, redox conditions, colloids/microbes/organics, rock matrix etc). Evaluation of these data, together with the latest status of the equivalent geological and hydrogeological site descriptive models, will therefore include an updating of the Hydrogeochemical Site Descriptive Model version 1.

In contrast to the input information available for the initial evaluation, the second evaluation will have access to:

- additional and more specialised groundwater data and their interpretation,
- a greater understanding of the important hydrogeochemical processes (e.g. reactions vs mixing),
- a greater understanding of the residence time and origin of the groundwaters,
- a greater understanding of the evolution of the ‘undisturbed’ groundwater environment,
- a greater understanding of the role of palaeohydrogeochemical reactions/mixing processes,
- a greater understanding of fracture geometry and mineralogy,
- a greater understanding of borehole hydraulics,
- a more developed Hydrogeological Site Descriptive Model version 1,
- a more developed Geological Site Descriptive Model version 1,
- a preliminary Hydrogeochemical Site Descriptive Model version 1.

Input data

Input data will comprise:

- results from the initial hydrogeochemical evaluation stage,
- specialised isotope evaluation/data,
- specialised redox evaluation/data,
- specialised colloid evaluation/data,
- specialised microbe evaluation/data,
- specialised gas evaluation/data,
- specialised organic evaluation/data,
- specialised rock matrix fluid evaluation/data,
- additional groundwater field and analytical data,
 - long-term monitoring data,
 - possible re-sampling/re-measurements at specific borehole locations,
 - possible new sampling/measurements at specific borehole locations,
- additional low transmissive rock matrix fluids/groundwaters,
- updated fracture mineralogy,
- latest Hydrogeochemical Site Descriptive Model version 1,
- latest Geological Site Descriptive Model version 1,
- latest Hydrogeological Site Descriptive Model version 1,
- associated uncertainties.

The reference to additional field and analytical data covers the on-going nature of the site investigations (e.g. long-term hydrochemical monitoring data) and, based on the initial hydrogeochemical evaluation, also the possibility to confirm existing data or gather additional data from new strategic sampling locations if deemed necessary. It is not foreseen that new boreholes will be drilled between the initial and second hydrogeochemical evaluation stages.

Evaluation of data

This second evaluation stage, based on the additional input data, will essentially update, modify, quantify and expand the preliminary results from the initial evaluation stage. In common with the initial evaluation stage, the following steps will be readdressed:

- quality control,
- chemical trends,
- hydrogeochemical modelling,
- conceptualisation,
- visualisation.

Quality control

In terms of quality control, the input from the specialised evaluations might reveal additional uncertainties concerning some of the input data from the initial hydrogeochemical evaluation. This may warrant some modification of the hydrogeochemical database which in turn may influence some of the modelling results.

Improvements resulting from new measurements may help to reduce/constrain the uncertainties described under the initial evaluation stage.

Chemical trends

This will comprise updating and modifying the results from the initial hydrogeochemical evaluation using the same approach as outlined in the initial evaluation stage.

Improvements resulting from new measurements may help to reduce/constrain the uncertainties described in the initial evaluation stage.

Modelling

This will comprise updating and modifying the results from the initial hydrogeochemical evaluation using the same approach as outlined in the initial evaluation stage.

Improvements resulting from new measurements may help to reduce/constrain the uncertainties described in the initial evaluation stage.

Conceptualisation

This will involve updating and modifying the preliminary Hydrogeochemical Site Descriptive Model version 1 resulting from the initial hydrogeochemical evaluation. The most important modifications will reflect:

- additional information from each of the specialised studies and how this will:
 - modify the groundwater dataset,
 - modify the lateral and vertical groundwater chemical and isotopic trends,
 - identify/confirm those areas dominated/influenced by microbially-mediated reactions,

Note: These data will be restricted spatially since they will mostly originate only from the 1–2 prioritised hydrogeochemical boreholes.

- groundwater chemistry from the rock matrix,
- M3 mass balance and mixing modelling based on a larger and more representative groundwater dataset,
- geochemical equilibrium rock/water interaction modelling based on a larger and more representative groundwater dataset,
- more detailed input from the hydrogeological modelling leading to:
 - major groundwater flow directions (site-scale: medium to high hydraulically conducting fractures and fracture zones),
 - minor groundwater flow directions (borehole/block-scale: single, low hydraulically conducting fracture zones),
 - potential information on the hydraulic character of the rock matrix.

At this stage the data available may allow a more elaborate modelling approach, for example the use of groundwater flow and transport simulations to calculate the potential distributions of the groundwater bodies, and not just restricted to modelling the groundwater flow directions which is no more than a qualitative integration of hydrogeochemistry and hydrodynamics. A series of simulations could be made to test different hypotheses, for example, to establish whether the system is steady-state or transient or to test different boundary conditions. The simulations are then compared with the actual groundwater composition.

Improvements resulting from new measurements may help to reduce/constrain the uncertainties described in the initial evaluation stage.

Visualisation

The preliminary Hydrogeochemical Site Descriptive Model (version 1) resulting from the initial hydrogeochemical evaluation will be updated to a modified version 1 (Table 2-1; Figure 5-1). Furthermore, with the potential addition of detailed borehole hydraulics (and associated preliminary hydrodynamic modelling) it should be possible to represent, at least schematically, the major and minor groundwater flow directions and the associated variations (due to mixing and/or water/rock reactions) in groundwater chemistry within the bedrock. For illustration, schematic visualisations based a manual approach and expert judgement will be used in all steps of the modelling along similar lines as that attempted by /Smellie and Laaksoharju, 1992/, /Bath et al, 2000, Figure 4-6/ and also within the Posiva site investigation studies /e.g. Pitkänen et al, 1999/.

Improvements resulting from new measurements may help to reduce/constrain the uncertainties described in the initial evaluation stage.

Output data

The major output from the ‘Second Hydrogeochemical Evaluation’ stage will be:

- a second iteration of hydrochemical data (representative/uncertainty evaluation),
- a second iteration of groundwater end members and degree of mixing using M3,
- a second iteration of rock/water reactions using PHREEQC,
- an updated Hydrogeochemical Site Descriptive Model version 1 (site-scale and borehole/block-scale),

- an updated understanding of the palaeohydrogeochemistry,
- a possible insight into the spatial distribution of groundwater chemistry from low transmissive domains and the rock matrix,
- an updated evaluation of uncertainties.

5.2.5 Refined hydrogeochemical evaluation

Provision has been made in the hydrogeochemical evaluation for additional refinement (Figure 5-1) resulting in a more complete Hydrogeochemical Site Descriptive Model version 1.

Input data

Input data will comprise:

- results from the second hydrogeochemical evaluation stage,
- possible additional groundwater analytical data (remeasurements; delayed analyses etc),
- possible additional data from the specialised studies,
- hydrogeochemical database modified to reflect representative values (i.e. minimum uncertainties),
- latest Hydrogeochemical Site Descriptive Model (version 1),
- latest Geological Site Descriptive Model (version 1),
- latest Hydrogeological Site Descriptive Model (version 1),
- associated uncertainties.

Evaluation of data

This refinement stage will essentially update and modify the results from the second hydrochemical evaluation stage by once again systematically addressing:

- quality control,
- chemical trends,
- modelling,
- conceptualisation,
- visualisation.

During this refined evaluation stage it is expected that only minor adjustments, if any, will be necessary to the above task list. The main refinement most probably will focus on the Hydrogeochemical Site Descriptive Model and this will depend on information from, in particular, the latest versions of the geological and hydrogeological site descriptive models.

Output data

The output from the 'Refined Hydrogeochemical Evaluation' stage will be:

- an updated version of the hydrogeochemical evaluation database (representing reasonably well tested and quantified uncertainties),
- a updated confirmation/modification of groundwater end-members and their degrees of mixing using M3,
- an updated confirmation/modification of rock/water reactions using PHREEQC,
- an update of specialised study areas,
- an updated evaluation of uncertainties,
- an updated understanding of the palaeohydrogeochemistry,
- an updated Hydrogeochemical Site Descriptive Model (version 1) based on the availability of the latest input from the geological and hydrogeological site descriptive models (version 1).

6 Documentation

6.1 Background

Documentation will be in the form of a written report together with a detailed record of the various steps fulfilled in the construction of the Hydrogeochemical Site Descriptive Model. These details are contained in an overall activity plan which defines the major aims, the steps involved to achieve these aims, the methodology to be employed, the expected output data and the time schedules to be met. Activities prior, during and subsequent to execution of the model construction will be documented, including when deviation from the activity plan has occurred.

In this context the recent approach employed at Laxemar has been used as a good example ('Testing the Methodology for Site Descriptive Modelling: Application for the Laxemar area' by /Andersson et al, 2002/), providing important proven experience which has helped considerably in organising the documentation approach presented below.

6.2 General flowchart

Hydrogeochemical evaluation is not always a straight forward task where well-defined detailed schemes can be followed rigorously. The work is generally determined by the available data, its quality and the purpose of the modelling exercises. For site investigations the modelling steps described in Chapter 5 have been defined in order to meet the requirements stated by SKB and the authorities. Furthermore, this modelling strategy and the various modelling steps have been tested in various SKB projects over the years and there is high degree of confidence in application and interpretation. What is presented in this chapter is a summary flow chart (Figure 6-1) which attempts to:

- integrate the various steps involved in hydrogeochemical modelling and how these activities relate to the field investigations,
- demonstrate how the hydrogeochemical evaluation is integrated with other modelling work such as geology and hydrogeology,
- indicate how the data are delivered and archived into the SKB database SICADA,
- and d) show how the information is used in the site characterisation analysis and repository design work.

Letters A–D in Figure 6-1 indicate the consecutive steps in the various activities, where A = the Descriptive/Conceptual Model, B = the Data Delivery, C = represents the Hydrogeochemical Site Descriptive Model versions x.x etc, and D = the Reporting of the hydrogeochemical evaluations/simulations.

6.3 Detailed documentation of the modelling work

The execution of the groundwater modelling work is detailed in an activity plan which requires approval by SKB before commencement of the work (see Tables 6-1, 6-2, 6-3 and 6-4). The activity plan defines the major aims, the steps involved in their achievement, the methodology to be employed, the expected output data and the time schedules. It consists of the following tables: a) Activity Table, b) Controlling Activity Table, c) Reporting Activity List, and d) Non-Conformance Report. The aims of these documents are to make sure that the required modelling steps are followed and that the quality assurance routines are met concerning traceability of the modelling steps and the key deliveries.

6.3.1 Activity Table

In practical terms the Activity Table (Table 6-1) outlines the major activities relating to the construction of a Hydrogeochemical Site Descriptive Model. The emphasis here is on close coordination within the 'Hydrogeochemical Analysis Group' such that all data are closely evaluated and documented using expert experience and judgement in parallel with mathematical or statistically-based modelling approaches.

6.3.2 Controlling Activity Table

The objective of the Controlling Activity Table (Table 6-2) is to control the activities and to document the procedures. Prior to execution of the modelling work the following are required to be defined: 1) Name of the Activity, 2) Input Data, 3) Controlling Documents, 4) Results/Deliveries, 5) Man Hours required for each activity, 6) Responsible Person in charge, and 7) Milestones.

6.3.3 Reporting Activity List

The Reporting Activity List (Table 6-3) has to be filled in during the execution of the activities. For the modelling work this form is to be completed by the Project Leader and should always be attached and accompany the Activity Plan.

6.3.4 Non-conformance Report

The Non-Conformance Report (Table 6-4) must be attached and filled in during execution of the activity in the event of a non-conformance from the approved Activity Plan. (See intranet, Management Systems, Non-Conformance; Separate Word-Template). Any non-conformance is to be reported to the Project Leader responsible for the modelling activity.

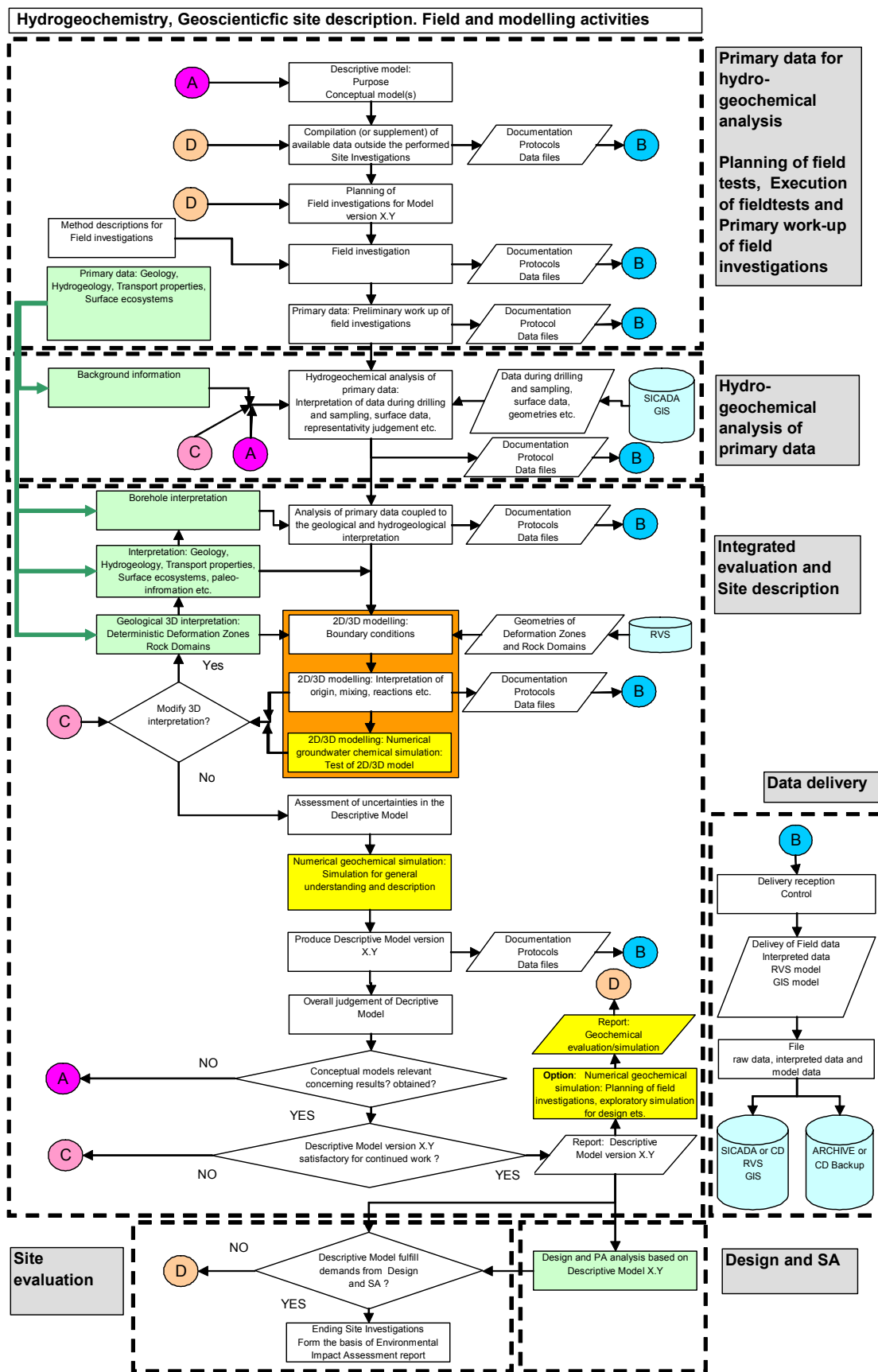


Figure 6-1. General flowchart (modified after I Rhén, pers comm, 2002) presents the overall approach to groundwater modelling work in relation to activities such as field work, data collection, modelling work and information such as geology and hydrogeology, how the data delivery is organised and how the information will be used in site evaluation. A–D in the flowchart (see Section 6.2 for explanation) indicates the consecutive steps in the various activities.

Table 6-1. Major activities related to constructing a Hydrogeochemical Site Descriptive Model

ID	Activity	Description
1	Meetings and planning	Regular project meetings with updating on on-going work and planning of future work
2	Data collection from SICADA and table construction	Compiling chemistry data tables for familiarisation and future modelling purposes
3	Evaluation of data; representative vs uncertain	Judgement of which samples will be used for further modelling
4	Manual evaluation/modelling of data	Scatter plots or models used for explorative/scoping analysis of the data
5	3D visualisation of measured data	Visualisation of measured chemical properties in 3D volume
6	Producing an initial conceptual model of the site	Model which describes the distribution of the groundwaters, their origin and degrees of mixing
7	Massbalance calculations	Calculations of the saturation state of the groundwater in relation to rock minerals
8	Mixing calculations and modelling	Calculate which mixing or reactive processes have affected the groundwater Modelling of mixing processes and reaction types
9	3D visualisation of modelled values	Show the distribution of calculated chemical properties of the rock in 3D
10	Up-dated conceptual model for the site	Updated model to describe the origin or the evolution of the groundwater
11	Compare and integrate with independent modelling	Compare the Hydrochemical Site Descriptive Model with, e.g. the Hydrogeological Site descriptive Model
12	Reporting	Compiling the information
13	External consultancies and review	Assessment of the results using expert knowledge and experience

Table 6-2. Controlling Activity Table – (AP ID F117-02-31)

ID	Activity	Input data	Controlling document	Results/Deliveries Reporting document	Time period/ Man-hours	Responsible	Comments/Milestones
7	<i>States what is to be executed</i>	<i>States what data are needed to be able to execute the activity</i>	<i>States reference number/ chapter where it says how the activity is to be executed. (NOTE that references should be unique)</i>	<i>States what results are to be delivered after completion of the activity and how they are to be reported (e.g. by indicating the reference no. of protocols to be filled in)</i>	<i>States time period and/or estimated amount of time required for the activity</i>	<i>States who is responsible for execution</i>	
1.	Meetings and planning		Project description and the activity plan	Project meeting protocols			
2.	Data collection from SICADA and table construction	Chemistry data from SICADA	Activity plan	Table in the final report, Excel file			
3.	Representativity evaluation of data	Chemistry data from SICADA	Activity plan	Table in the final report, Excel File			
4.	Manual evaluation/ modelling of data	Chemistry data from SICADA	Project description and the activity plan	Chapter in the final report			
5.	3D visualisation of measured data and input data from the geological structural model	Chemistry data from SICADA	Project description and the activity plan	Descriptive model and pictures in the final report			
6.	Producing a conceptual model of the site	Output of ID 4 and 5	Project description and the activity plan	Descriptive model and pictures in the final report			
7.	Massbalance calculations	Output of ID 4	Project description and the activity plan	Table and chapter in the report, Excel File			
8.	Mixing Calculations	Output of ID 4	Project description and the activity plan	Chapter in the final report, Excel file			
9.	3D visualisation of modelled values	Output of ID 8	Project description and the activity plan	Descriptive model and picture in the final report			
10.	Updated conceptual model for the site	Output of ID 7 and 8	Project description and the activity plan	Chapter in the final report			
11.	Compare and integrate with independent modelling	Own and other modelling such as hydromodelling	Project description and the activity plan	Chapter in the final report			
12.	Reporting	Output of ID 2 to 11	Project description and the activity plan	Chapters in the final report, CD			
13.	External consultancies and review	Expert knowledge		Editions of the chapters and updating of the modelling in the final report, CD			
Prepared by:					Approved by.		
_____					_____ Date: _____		

Table 6-3. Reporting Activity List

ID	Activity	Input data	Controlling document	Results/Deliveries Reporting document	Task completed	Comments	Delivery received	Archiving	Signature/ date
	<i>Copy from controlling table + any additions</i>	<i>Copy from controlling table + any additions</i>	<i>Copy from controlling table + any additions</i>	<i>Copy from controlling table + any additions</i>	<i>Signature of person who executed or is responsible for execution</i>		<i>Signature of responsible person that everything is delivered acc. to Activity Plan</i>	<i>Indication where reported results are archived</i>	<i>Signature that reported results are archived</i>
1	Meetings and planning		Project description and the activity plan	Project meeting protocols					
2	Data collection from SICADA and table construction	Chemistry data from SICADA	Activity plan	Table in the final report, Excel file					
3	Representativity evaluation of data	Chemistry data from SICADA	Activity plan	Table in the final report, Excel File					
4	Manual evaluation/modelling of data	Chemistry data from SICADA	Project description and the activity plan	Chapter in the final report					
5	3D visualisation of measured data	Chemistry data from SICADA	Project description and the activity plan	Descriptive model and pictures in the final report					
6	Producing a conceptual model of the site	Output of ID 4 and 5	Project description and the activity plan	Descriptive model and pictures in the final report					
7	Massbalance calculations	Output of ID 4	Project description and the activity plan	Table and chapter in the report, Excel File					
8	Mixing calculations	Output of ID 4	Project description and the activity plan	Chapter in the final report, Excel file					
9	3D visualisation of modelled values	Output of ID 8	Project description and the activity plan	Descriptive model and picture in the final report					
10	Updated conceptual model for the site	Output of ID 7 and 8	Project description and the activity plan	Chapter in the final report					
11	Compare and integrate with independent modelling	Own and other modelling such as hydromodelling	Project description and the activity plan	Chapter in the final report					
12	Reporting	Output of ID 2 to 11	Project description and the activity plan	Chapters in the final report, CD					
13	External consultancies and review	Expert knowledge		Editions of the chapters and updating of the modelling in the final report, CD					
Tasks completed (<i>results/products including any non-conformance reports etc delivered</i>):						Approved by: <i>Date and signature of purchaser of activity (project manager)</i>			

Table 6-4. Non-Conformance Report

Typ	<input type="checkbox"/> Kvalitet	<input type="checkbox"/> Säkerhet	<input type="checkbox"/> Miljö	<input type="checkbox"/> Arbetsmiljö	<input type="checkbox"/> Kärnsäkerhet
Registreras i G:/KS/Cert2000/Erfarenheter/Avvikelser.xls. (Tillbud och olyckor m.a.p. personsäkerhet och hälsa rapporteras på särskilt formulär)					
Utfärdad av					
.....
Handläggare	Datum	Namnteckning			
Ev. kund					
.....					
Projekt/process/verksamhet (anges om möjligt)					
.....					
Krav i rutin/handbok eller beskrivning (anges om möjligt)					
Avvikelse			Ursprunglig handling/bilagor		
Troliga konsekvenser av avvikelsen					
Förslag till (kortsiktig) åtgärd för att eliminera avvikelsen					
Åtgärd för att eliminera avvikelsen godkänd					
.....
Ansvarig	Datum	Namnteckning			
Åtgärd enligt ovan utförd					
.....
Handläggare	Datum	Namnteckning			
Förslag till korrigerande åtgärd för att förhindra upprepande (eliminera orsaken)					
Åtgärd för att eliminera avvikelsen godkänd					
.....
Ansvarig	Datum	Namnteckning			
Åtgärd enligt ovan utförd och befunden tillräcklig					
.....
Handläggare	Datum	Namnteckning			
Förslag till eventuell förebyggande åtgärd för att förhindra att andra typer av avvikelser uppkommer					
Förebyggande åtgärd godkänd					
.....
Ansvarig	Datum	Namnteckning			
Åtgärd enligt ovan utförd					
.....
Handläggare	Datum	Namnteckning			

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8 Acknowledgements

Many scientists working within the SKB Hydrogeochemical Programme during the last 15–20 years have contributed indirectly to this document and are hereby acknowledged. Those not included in the author list but who have contributed directly within their respective areas of speciality are Karsten Pedersen (Microbes; Organic Carbon; Gases), Ignasi Puigdomenéch (Redox) and Ann-Chatrin Nilsson (Analytical Programme). The content of the document has benefited greatly from periodic reviews by Peter Wikberg, Anders Ström, Johan Andersson and Nils-Åke Larsson, and finally from the two external reviewers, Mel Gascoyne and Bill Wallin.