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Task force on modelling of groundwater flow and transport of solutes

Task 5 Summary report

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Abstract

The Äspö Hard Rock Laboratory (HRL) is located in the Simpevarp area, southeast Sweden, some 35 km north of Oskarshamn. Construction of the underground laboratory commenced in 1990 and was completed in 1995, consisting of a 3.6 km long tunnel excavated in crystalline rock to a depth of approximately 460 m. Prior to, during and subsequent to completion, research concerning the deep geological disposal of nuclear waste in fractured crystalline rock has been carried out. Central to this research has been the characterisation of the groundwater flow system and the chemistry of the groundwaters at Äspö prior to excavation (Pre-investigation Phase) and subsequently to monitor changes in these parameters during the evolution of laboratory construction (Construction Phase).

The principle aim of the Äspö Task 5 modelling exercise has been to compare and ultimately integrate hydrogeochemistry and hydrogeology using the input data from the pre-investigation and construction phases. The main objectives were:

- to assess the consistency of groundwater-flow models and hydrogeochemical mixing-reaction models through integration and comparison of hydraulic and hydrogeochemical data obtained before and during tunnel construction, and
- to develop a procedure for integration of hydrological and hydrogeochemical information which could be used for disposal site assessments.

Task 5 commenced in 1998 and was finalised in 2002. Participating modelling teams in the project represented ANDRA (France; three modelling teams – ANTEA, ITASCA, CEA), BMWi/BGR (Germany), ENRESA (Spain), JNC (Japan), CRIEPI (Japan), Posiva (Finland) and SKB (Sweden; two modelling teams – CFE and Intera (now GeoPoint)).

Experience from Task 5 has highlighted several important aspects for site investigations facilitating the possibilities for mathematically integrated modelling and consistency checks that should be taken into account for future repository performance assessments.

Equally important is that Task 5 has provided the opportunity to bring together two scientific disciplines which have traditionally tended to work in parallel rather in collaboration. This is an important first step. The process of understanding, interacting and integrating has now been initiated and, given more time and resources, the degree of scientific integration would have been greater. There is now a much stronger appreciation that the use of hydrogeochemistry can lead to an increased understanding of hydrogeology and *vice-versa*.

Sammanfattning

Äspölaboratoriet är lokaliserat i Simpevarpsregionen i sydöstra Sverige, ca 35 km norr om Oskarshamn. Byggandet av underjordslaboratoriet, som påbörjades 1990 och färdigställdes 1995, består av en 3.6 km lång tunnel utsprängd och borrad i kristallin berggrund ner till ett djup av ca 460m. Innan, under och efter färdigställandet av laboratoriet har forskning genomförts som rör djupförvar av kärnavfall i kristallin berggrund. Centralt för denna forskning har varit karakteriseringen av grundvattenflödessystemet och grundvattenkemin vid Äspö innan tunnelbygget (Förundersökningsfas) och att därefter monitera dessa parametrar under byggandet av laboratoriet (Konstruktionsfas).

Huvudsyftet med Äspö Task 5 modelleringen har varit att jämföra och integrera hydrogeokemi och hydrogeologi genom att använda data från förundersöknings- och konstruktionsfaserna. Huvudsyftena var:

- att bedöma konsistensen mellan grundvattenflödesmodellerna och hydrogeokemiska blandningsmodeller genom integrering och jämförelse av hydrogeologiska och hydrogeokemiska data samlade före och under byggandet av laboratorietunnel och
- att utveckla en procedur för integrering av hydrogeologi och hydrogeokemisk information vilket skulle kunna nyttjas vid bedömning av en plats för ett djupförvar.

Task 5 påbörjades 1998 och slutfördes 2002. Deltagande modelleringsgrupper I projektet representerade ANDRA (Frankrike; tre modellgrupper – ANTEA, ITASCA, CEA), BMWi (Tyskland), ENRESA (Spanien), JNC (Japan), CRIEPI (Japan), Posiva (Finland) and SKB (Sverige; två modellgrupper – CFE och Intera (nu GeoPoint)).

Erfarenheterna från Task 5 har visat på flera viktiga aspekter för platsundersökningarna som rör möjligheterna för integrerade matematiska modeller och konsistenskontroller som bör göras vid framtida bedömningar av platser för ett djupförvar.

Lika betydelsefullt har varit att Task 5 gett möjligheten att sammanföra två vetenskapliga discipliner vilka traditionellt vanligen arbetat parallellt istället för tillsammans. Det projektet har varit ett första steg. Denna process för förståelse, interagerande och integrerande har nu startats och, med mer tid och resurser, skulle den vetenskapliga integreringen ha blivit större. Det är idag en mycket större förståelse att användandet av hydrogeokemi kan medföra en större förståelse av hydrogeologi och viceversa.

Executive Summary

Introduction

The Äspö Hard Rock Laboratory (HRL) is located in the Simpevarp area, southeast Sweden, some 35 km north of Oskarshamn. Construction of the underground laboratory commenced in 1990 and was completed in 1995, consisting of a 3.6 km long tunnel excavated in crystalline rock to a depth of approximately 460 m (*Figure 1*). Prior to, during and subsequent to completion, research concerning the deep geological disposal of nuclear waste in fractured crystalline rock has been carried out. Central to this research has been the characterisation of the groundwater flow system and the chemistry of the groundwaters at Äspö prior to excavation (Pre-investigation Phase) and subsequently to monitor changes in these parameters during the evolution of laboratory construction (Construction Phase). There was, therefore, a considerable amount of available data for modelling purposes compiled over a 15 years period.

To successfully understand and model the groundwater flow and hydrogeochemistry of a potential radioactive waste site is important since these two processes will play a central role in determining potential radionuclide transport pathways from the repository to the biosphere in the event of leakage from one or more defective canisters. It is quite clear that to integrate the two disciplines would give greater confidence in describing present groundwater conditions and consequently predicting future repository conditions.

The major aim of Task 5 was, therefore, to integrate hydrogeochemistry and hydrogeology. The proposed Task 5 modelling was also expected to be useful for a future assessment of the stability of the hydrodynamic and hydrogeochemical conditions at Äspö. This modelling approach could then be used for any future repository site investigations, especially in a fractured crystalline bedrock environment.

Task 5 commenced in 1998 and was finalised in 2002. Participating modelling teams in the project represented ANDRA (France; three modelling teams – ANTEA, ITASCA and CEA), BMWi/BGR (Germany), ENRESA (Spain), JNC (Japan), CRIEPI (Japan), Posiva (Finland), and SKB (Sweden; two modelling teams – CFE and Intera (now GeoPoint)). Funding organisations:
Svensk Kärnbränslehantering AB (SKB), Sweden,
Power Reactor & Nuclear Fuel Development Corporation (JNC), Japan
Central Research Institute of Electric Power Industry (CRIEPI) Japan
Agence National Pour la Gestion des Déchets Radioactifs (ANDRA), France
POSIVA Oy, Finland
Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie (BMW), Germany
Empresa Nacional de Residuos Radiactivas (ENRESA), Spain

Geological and hydrogeological setting

The island of Äspö comprises a slightly undulating topography of well exposed rock with a maximum elevation of about 14 m, characterised by small drainage basins with some peatlands and sediments in the topographic lows. There are no perennial streams on the island, the surface water being drained to the Baltic Sea by the peatlands, sediments or directly to the sea. West of Äspö island, on the Laxemar mainland area, discharge areas occur along the coast but also in peatlands and along small streams flowing towards the Baltic sea. The annual mean precipitation and temperature of the area are about 550 mm/year and 6.5°C respectively, with the annual sea level fluctuations generally within ± 0.5 m. The groundwater table elevation above the mean sea level is about 30% of the elevation of the topography above mean sea level, within a few hundred metres from the coastline.

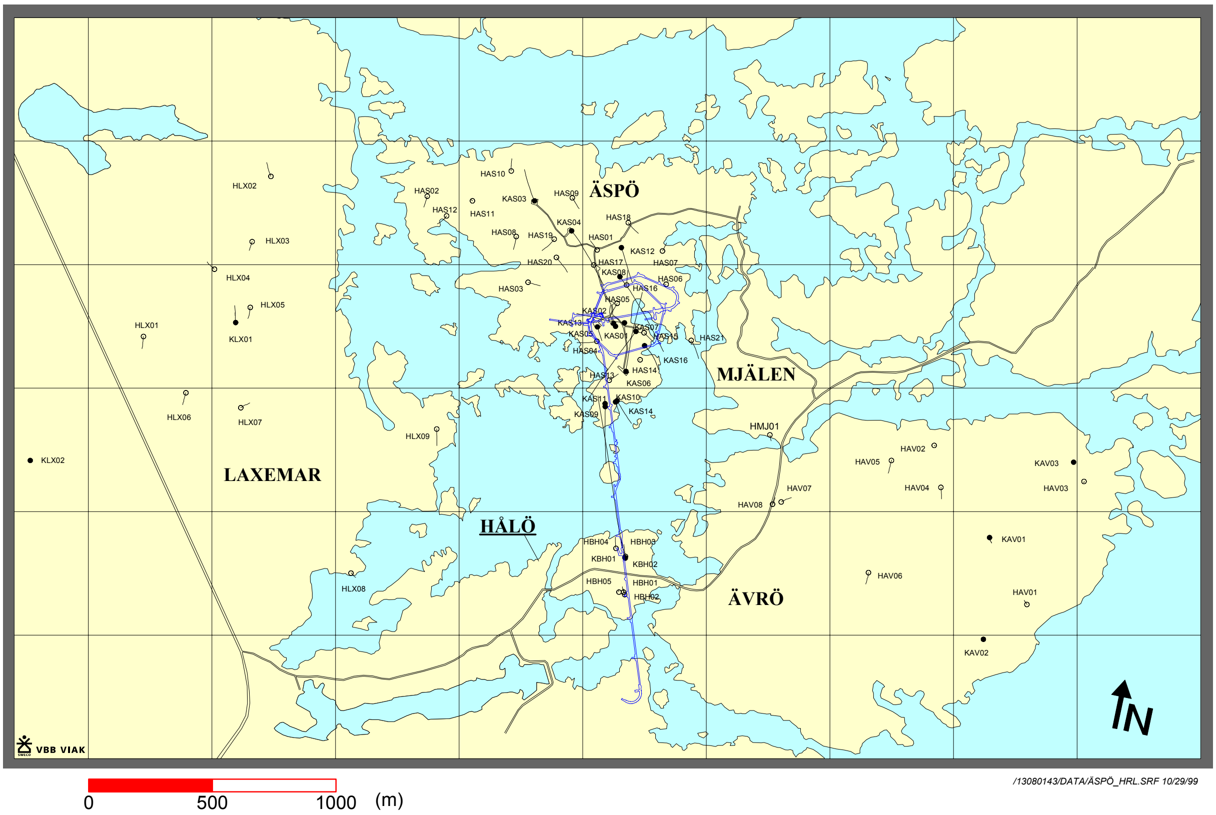


***Figure 1**. Location of the Äspö Hard Rock Laboratory (HRL).*

The geology is characterised by a red to grey porphyritic granite-granodiorite of Småland type, containing microcline megacrysts up to 1 to 3 cm in size. To the south of the island a redder granite variety, the Ävrö 'true' granite outcrops, containing small (<1 cm) sparsely distributed microcline megacrysts. Within the granite are east-west trending lenses/sheets of fine-grained granite and also greenstone (metabasalt), which are usually strongly altered. Subordinate lenses of fine-grained grey metavolcanites (of dacitic composition) also occur. Both of these rock types predate the Småland granite. Finally, small occurrences of pegmatite commonly occur as very narrow dykes (decimetres in size).

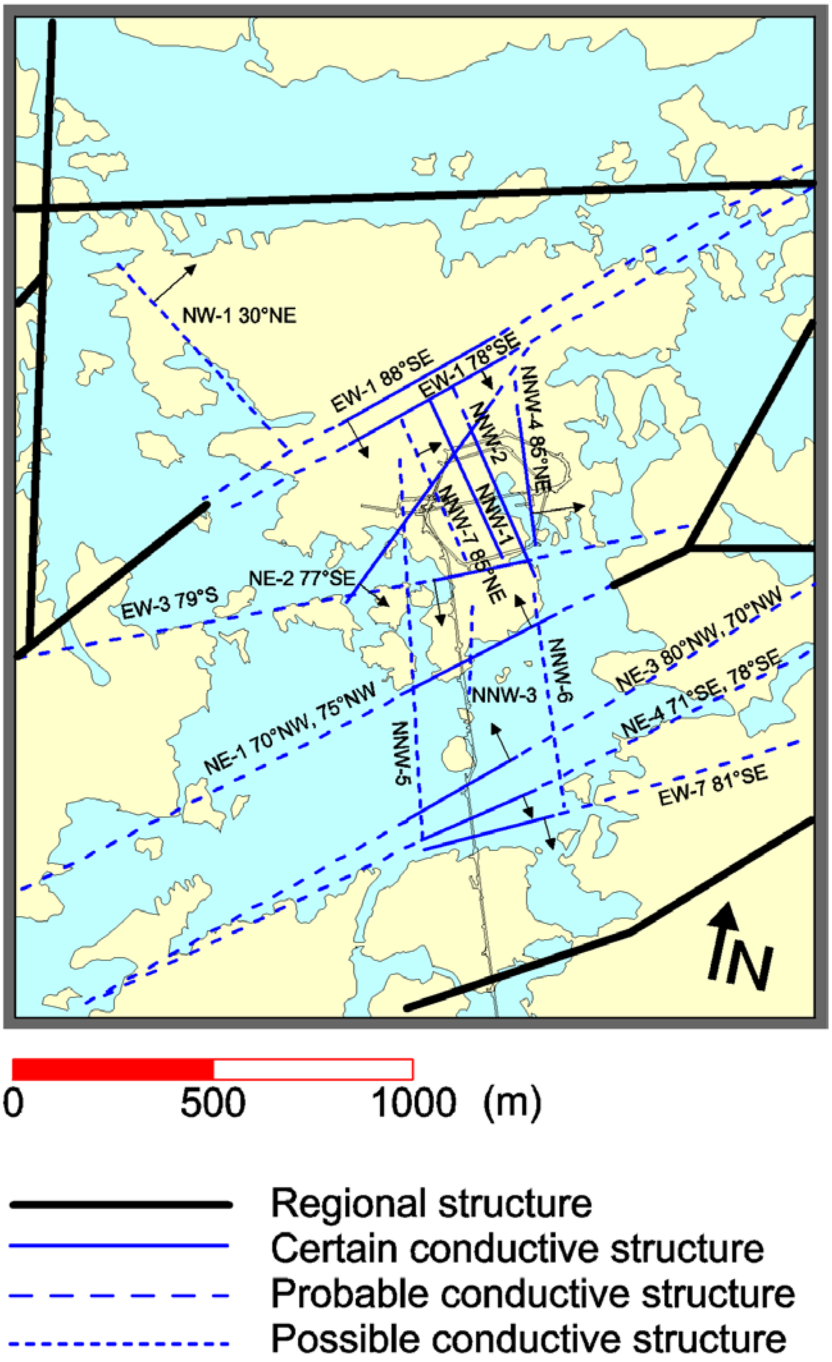


Figure 2. *Major structural subdivisions and hydraulic conductors of Äspö island and its vicinity.*

Structurally, Äspö island is divided into two main blocks by a NE-trending regional shear zone (EW-1); this reflects the main structural anistropy of the island which is parallel to an almost vertical, more or less penetrating foliation trending NE-ENE (*Figure 2*). In both blocks the Småland granite, with associated greenstones and fine-grained granite/aplite varieties, dominates, although in the southern block below 300 m, more basic dioritic varieties of the Småland granite (i.e. Äspö diorite) begin to dominate.

The EW-1 shear zone, which is vertical to subvertical to the north, consists of strongly foliated heterogeneous Småland granite containing a large number of mylonitic lenses and greenstone xenoliths. Highly fractured zones (5-10 m wide), alternating with more normally fractured rock, complicate the shear structure that has also undergone substantial weathering, seen as oxidation of magnetite to haematite and Fe-oxyhydroxides. This explains the negative aeromagnetic anomaly detected during the reconnaissance phase of the investigations.

The northern block is more fractured than its southern counterpart; in both cases the fractures are vertical to sub-vertical in orientation. One important group of discontinuous subhorizontal zones occurs at depths of 300-500 m.

The main fracture filling mineral phases consist of, in decreasing order of frequency: group A (chlorite, calcite), group B (haematite, Fe-oxyhydroxides, epidote, fluorite), and group C (pyrite, magnetite, laumonite/prehnite, gypsum).

The areal distribution of hydraulic conductivity at Äspö on the site scale is heterogeneous. Generally the fine-grained granite/aplite tends to be the most conductive unit, probably because it is the most competent rock type and is therefore inclined to fracture easily in response to tectonic movement. The increased fracture frequency in the northern block of Äspö reflects a correspondingly higher hydraulic conductivity. Furthermore, there is also a general decrease in the variability of hydraulic conductivity with depth.

Recharge/discharge and groundwater flow through Äspö is controlled by the major tectonic fractures and discontinuities with a general groundwater flow trend, at least in the upper 500 m or so, from north to south towards the NE-1 zone, facilitated by the NNW-trending vertical to subvertical fractures. The major E-W trending shear zone (EW-1) is a strong recharge feature. Following tunnel construction the main groundwater flow is from the south, but the drawdown of meteoric water from shallower levels, in addition to minor inputs from the north via EW-1 and the NNW-trending fractures, also occurs towards the tunnel.

Sources of data

Site-derived data

Investigations at the Äspö HRL fall into three categories: 1) Pre-investigation Phase (1986-1990), 2) Construction Phase (1990-1995), and 3) Operation Phase (1995-2050?). The Task 5 modelling exercise centred on data accumulated during the pre-investigation and construction phases.

The ‘Pre-investigation Phase’, extending from the surface to around 1000 m, was aimed at siting the laboratory, describing the natural hydrogeological, hydrochemical and geochemical conditions in the bedrock, and predicting the changes that will occur during the excavation and construction of the underground laboratory. This phase was extremely important in that it provided the only opportunity to study the natural, ‘undisturbed’ groundwater conditions in the bedrock, in particular to provide a reliable reference point for all subsequent hydrogeological and hydrogeochemical investigations carried out during the construction and operation phases.

Following the pre-investigation phase, construction of the access tunnel and underground facilities (‘Construction Phase’) commenced. The maximum depth of the laboratory is 460 m and the tunnel has a total length of 3 600 m. During this phase extensive investigations, tests and experiments were carried out in parallel with the excavations. The focus of the experimental work was mainly to check the reliability of interpretations based on the pre-investigation phase and to broaden and detail the database of the Äspö site. The first part of the tunnel to 3 200 m was excavated using the drill-and-blast technique and the final 400 metres using the Tunnel Boring Machine (TBM) with a diameter of 5 metres.

Hydraulically the Äspö site consists of Hydraulic Conductive Domains (HCDs) and Hydraulic Rock Mass Domains (HRDs). The former represent fractures zones (> 5 m in width) and have generally a substantial storage capacity, and the latter includes single fractures and minor fracture zones with a lower effective hydraulic conductivity than the HCDs but still with a substantial storage capacity.

The hydrogeological and hydrogeochemical impact of the tunnel construction was continuously monitored from some of the pre-investigation boreholes, from probe holes drilled at the tunnel face during advancement of the excavations, and from strategically located control points along the completed tunnel representing the intersection of the tunnel with hydraulically active fracture zones (HCDs) and also from the low permeable rock mass (HRDs) between these zones. These monitored time-series data from the tunnel control points and some of the pre-investigation boreholes proved to be very important in the Task 5 modelling.

During these two phases of investigation conceptualisation of the site evolved as more data became available. This resulted in a series of model development stages which culminated in an integrated site-descriptive model of the undisturbed groundwater conditions from the pre-investigation phase, and of the disturbed groundwater conditions resulting from tunnel excavation. These models formed the basis to the Task 5 modelling exercise.

M3-derived data

Additional data made available to the modelling groups were the so-called M3-derived data. M3 stands for Multivariate Mixing and Mass balance and is a statistical method to analyse variations in groundwater compositions so that the mixing components, their proportions, and the effects from chemical reactions are revealed. The M3 method, being mathematically based, has the advantage of objectivity when classifying large sets of hydrochemical data, although the initial and final choice of groundwater end members requires close familiarity with the system being investigated. Further features of M3 include the fact that model construction is based on all the measured data and therefore all the samples are compared by using the same model, and that both conservative and non-conservative species are used. It should be noted, however, that the M3 model is only concerned with water comparison data and no space or time restraints, or geological and hydrogeological information, are included. The M3 modelling approach has been widely applied to the Äspö site at all stages of investigation.

Modelling

Background perspective and Task 5 issues

The principle aim of the Äspö Task 5 modelling exercise was to compare and ultimately integrate hydrogeochemistry and hydrogeology. The input data used were from the pre-investigation and construction phases. The main objectives were:

- to assess the consistency of groundwater-flow models and hydrogeochemical mixing-reaction models through integration and comparison of hydraulic and hydrogeochemical data obtained before and during tunnel construction, and
- to develop a procedure for integration of hydrological and hydrogeochemical information which could be used for disposal site assessments.

The rationale behind these modelling exercises was based on the following:

- groundwater flow and chemistry are important for the safety and performance assessment of a deep geological disposal of radioactive waste,
- if groundwater flow and chemistry are integrated properly, it should improve confidence in the description of present and future conditions at a potential repository candidate site, and
- the modelling approaches used in Task 5, if considered successful, could be used for ~~any~~ future repository site investigations especially in a fractured crystalline rock environment.

In order to facilitate comparison and integration of hydrogeology and hydrogeochemistry, the series of control points identified along the tunnel were ideal in that both hydraulic and hydrochemical parameters were routinely measured at each location. Based on these tunnel locations, a series of measures were identified to check the performance of the models. These performance measures were:

- the nature of the groundwater flow pattern through the bedrock to the tunnel control points
- the advective groundwater travel time distribution to the control points, and
- the nature of the groundwater chemical evolution to explain the results at each control point.

Two different modelling aims were specified: a) tunnel section 0-2900 m was chosen for model calibration and all pre-construction and construction data were made available, and b) tunnel section 2900-3600 m was chosen for model prediction where only the pre-investigation input data were made available; the objective was to predict the construction phase disturbance.

Hydrogeochemical modelling based on M3

Modelling, based mainly on the M3 approach, constituted the active hydrogeochemical contribution to Task 5 by SKB. It had a two-fold contribution:

- to fulfill SKB's contribution to the main Task 5 objective of integrating hydrogeochemistry with a hydrodynamic groundwater flow model, and
- to provide calculated groundwater mixing ratios from each control point to the other modelling groups to achieve some common ground for model comparison

The step-wise approach employed in the Task 5 modelling involved:

- selection of reference waters (or end members)
- testing the suitability of the M3 model
- modelling and visualising the changes in groundwater composition due to the tunnel construction (0-2900 m tunnel length)
- comparison of measured and calculated mixing proportions at selected control points (0-2900 m tunnel length)
- modelled predictions of mixing ratios at selected control points (2900-3600 m tunnel position)
- comparison of predictions at all control points (0-3600 m tunnel position)

The M3 hydrogeochemical modelling approach generated a data set of calculated groundwater mixing proportions for each of the selected control points. Comparison of the measured values with those calculated by M3 showed that mixing was the dominating process, and such data should be useful to calibrate and test the different hydrodynamic models used in Task 5, a central aim of the task.

Hydrodynamic modelling approaches, application and results

The modelled volumes chosen were approximately similar for all Task 5 modelling groups (2 x 2 x 1 km^3). The majority of the groups modelled only the Hydraulic Conductor Domains (HCDs) and did not consider a fully 3D model. A fully 3D model, including both HCDs and Hydraulic Rock mass Domains (HRDs), was used by ANDRA/ANTEA, CRIEPI, JNC/Golder, Posiva/VTT and SKB/CFE/Intera. The internal structure has generally been a continuum approach but one group used Channel Network for HCDs (ANDRA/ITASCA) and one group assumed constant properties for the HCDs and modelled the HRDs as a Discrete Fracture Network (JNC/Golder). However all models could show that the piezometric levels were comparable to the measured ones, but a rather large spread of final (calibrated) parameter values for the HCDs and HRDs for the different groups was noticeable, probably to some extent dependent on the choice of a fully 3D (or otherwise) modelling approach. A rather wide range for the kinematic porosities (or flow aperture) has been suggested for the HCDs from the different modelling groups.

Dispersion and diffusion were considered by some modelling teams but sorption/desorption were not considered relevant; matrix diffusion was considered by one team (Posiva/VTT).

Modelling of groundwater flow into the tunnel can be made in two ways: 1) distributing the measured flow rates as prescribed fluxes along the tunnel as a time dependent series, or 2) assuming atmospheric pressure in the tunnel and considering just a skin (hydraulic resistance) around the tunnel to obtain the measured flows. The modelling groups used one or the other of these methods and adopted different ways of carrying out the transient simulations; some made true transient simulations whilst others made step-wise stationary solutions of the pressure field for defined tunnel face positions.

All available data have not been used to test and calibrate the models. In addition, only limited sensitivity studies have been made; this was due to the limited resources (money and time) and the large amount of data that were supplied. In general:

- Most groups were successful in calibrating and testing their respective models to simulate the Äspö groundwater flow conditions.
- Hydrogeochemistry, in the form of single species or M3 mixing ratios, was used mainly to calibrate and modify properties of the Hydraulic Conductor Domains.
- The presence of flow paths to control points was to some extent shown and discussed. Only limited attempts were made to estimate the advective groundwater travel time distribution to the control points.

Hydrogeochemical modelling approaches, application and results

The use of hydrogeochemistry in modelling hydrodynamic flow conditions traditionally has been restricted to salinity/density input parameters, i.e. physical parameters easily integrated mathematically into the numerical models. A concerted effort therefore was made in Task 5 to expand the quantitative use of hydrogeochemistry. Since existing integrated codes are few, Task 5 provided the opportunity of modifying such models that exist or developing new model approaches. To establish some common ground and provide constraints on the modelling, SKB provided the modelling teams with M3 calculated groundwater end member mixing proportions for each of the control points. The modelling teams were also presented with a list of groundwater chemical reactions known to characterise the Äspö site and which may influence the groundwater chemistry during mixing; the teams were given the option to incorporate these reactions.

All modelling groups used the M3 calculated hydrochemical mixing ratios at control points to compare with the modelled hydrodynamic simulations; six out of the nine groups addressed the potential influence of chemical reactions on the groundwater chemistry during mixing. Note also that some groups (e.g. BMWi/BGR, CRIEPI, JNC/Golder and Posiva/VTT) used other approaches to calculate and compare mixing ratios with the M3 method, in particular Posiva/VTT and JNC/Golder who presented alternative methods from first principles.

In general:

- All groups treated the groundwater mixing ratios in the hydrodynamic simulations as conservative, i.e. assuming no water/rock reactions.
- Hydrogeochemical modelling was attempted by six out of the nine groups.
- Hydrogeochemical reaction modelling, assuming thermodynamic equilibrium conditions, was carried out by four groups. Generally this showed that certain reactions have some effect on the groundwater chemistry during mixing. The reaction types tended to be site-specific, i.e. organic decomposition leading to an increase of HCO_3 is microbially mediated and takes place under the landmass; sulphate reduction, also microbially mediated, occurs under the sea floor. Cation exchange by clay minerals is significant suggesting an exchange of Ca/Na for Mg/K; such reactions are restricted to the presence of clays/gouge material in fracture zones and not considered widespread in the Äspö bedrock.
- Hydrogeochemical reactions, whilst detectable, are largely overshadowed at Äspö when compared to groundwater mixing processes.

Integration of hydrodynamics and hydrogeochemistry

Since the principle aim of Task 5 was to integrate hydrogeochemistry with hydrogeology, one of the requirements from the modelling teams was to provide a flow chart showing how they intended (and actually accomplished) to integrate hydrogeochemical data into their respective hydrodynamic models. As an example, the intended approach of SKB/CFE was circulated to all participants.

The modelling groups used the SKB M3 hydrogeochemical end member mixing ratios as input to the hydrodynamic modelling exercise (e.g. initial and boundary conditions) and all models used the M3 calculated hydrogeochemical mixing ratios for each control point to compare modelled simulations (e.g. for calibration purposes). For example, JNC/Golder constructed a flow model which was then run with the initial boundary condition groundwater chemistry to provide hydrogeochemical simulations. Differences between measured and modelled hydrochemistry were used then to calibrate the hydrodynamic model. Furthermore, they considered the chemistry as pure mixing in the particle tracking carried out. ENRESA, ANDRA/CEA and ANDRA/ANTEA all used hydrogeochemistry to initial and boundary condition input and flow model calibration. The SKB/CFE integrated approach emphasised that it should be performed in two steps with a consistency check as the final event in both steps. In common with other teams, the consistency check compared the measured chemical composition (or mixing ratios) at each control point with the chemical composition (or mixing ratios) derived from the hydrodynamic modelling of the flow field. Modelling of the flow field incorporated input of flow, pressure, salinity/density and water end-member type.

The potential influence of hydrogeochemical reactions during groundwater mixing was carried out by six of the nine groups, with a more quantitative evaluation by four groups. BMWi/BGR emphasised the importance of chemical equilibrium reaction processes (particularly in the pre-investigation phase) together with mixing processes (dominating the construction phase) to explain the groundwater compositions at Äspö. The hydrodynamic modelling approach simulated flow and solute transport and the PHREEQC code was used to model the reaction chemistry. Both modelling approaches were carried out in two different steps that ~~had to be~~ were combined in succession. Finally, using the time-series measured groundwater compositions a hydrogeochemical model was established which was used to simulate the control point compositions. CRIEPI combined groundwater flow modelling with solute transport (constrained to conservative species, Cl and $\delta^{18}O$) and chemical reaction modelling using PHREEQE.

Coupled transport/hydrogeochemical simulations were performed in a limited region of the hydrodynamic model described by ANDRA/ITASCA. The modelling approach initially used the groundwater mixing ratios to better calibrate the hydrodynamic model; the coupled geochemical model assumed thermodynamic equilibrium conditions and only one potential chemical reaction was considered, that of carbonate dissolution/precipitation.

ENRESA/UDC did not hydrogeochemically model the influence of chemical reactions on the groundwater chemistry as part of the Task 5 exercise. However, outside the framework of the project they carried out numerical simulations on the Redox Zone, which intersects the access tunnel at 70 m depth. The simulations were carried out using the CORE^{2D} finite element code, a coupled groundwater flow and reactive solute transport model used to perform reactive transport simulations. In general, these simulations resulted in a good agreement between computed and measured concentrations (at a depth of 70 m). The coupled model was able to reproduce the observed behaviour of most dissolved species, however some discrepancies were found for dissolved bicarbonates and sulphates. Subsequent hydrobiogeochemical modelling showed these discrepancies to be the result of microbially-mediated processes.

In general, the main conclusions from the various integrated modelling approaches included:

- Simple simulation of mixing ratios (with or without chemical reactions) was used as a basis to calibrate (consistency check) the hydrogeological model
- Hydrogeochemical time-series data at the selected control points reflected changes in the hydrodynamic flow conditions and were useful therefore for calibration purposes.
- Use of salinity (density) data to simulate large-scale hydrodynamic flow conditions was considered essential by some groups.
- Coupled flow and multicomponent reactive transport modelling was carried out by two groups; this is an important area to be developed.
- Modelling and integration strategies were to some extent discussed and described.

Model uncertainties

All groups identified a number of different uncertainties in the final models presented and these uncertainties differed considerably between the groups. Partly it reflected the modelling approaches, but equally it reflected the difficulty of how to handle such a large quantity of data and find a structured, step-wise approach to build and test models using these data. However, the groups had one thing in common; all identified the problem of how to assess reasonable initial conditions based on a rather sparsely distributed data set, except for around the Äspö tunnel. Another problem was that the transient simulations indicated that after some years, groundwater from the vertical boundaries entered into the tunnel. The chosen size of the modelled volumes (about 2 x 2 x 1 km^3) was not large enough to avoid that effect.

The modeller's use of groundwater mixing proportions, and sometimes the chemical constituents, was considered to have improved confidence in the models constructed.

Alternative hydrogeochemical approaches

JNC/Golder and Posiva/VTT carried out independent methods to calculate the mixing proportions of reference end member waters and the sampled groundwaters. These serve as alternative approaches to the M3 calculations in different respects. The JNC/Golder approach is, in common with M3, statistically based and shares many similarities, but goes one step further in that selection of the chemical components (analogous to the M3 end members) and mixing proportion calculations are based on all the chemical variability of the dataset. This ensures a more objective choice of 'end members' and, in turn, increases confidence in the quality of the calculated groundwater mixing proportions. In contrast, the Posiva/VTT approach is not mathematically-based but has the great advantage of integrating chemical reactions; an obvious disadvantage is the necessity of substantial input of expert judgement.

These model developments reflect continued improvement in hydrogeochemical evaluation methodology that has been stimulated by the M3 modelling. M3, as with any modelling tool, has its weak points, but it is a quick and convenient method to initially classify large hydrogeochemical data sets given the Äspö type hydrodynamic groundwater environment. As pointed out by JNC/Golder, however, it may not be so suitable for shallow, fresh-water environments characterised by reactions rather then mixing. The Posiva/VTT methodology has its place in the detailed geochemical understanding of the groundwater flow system, but it can be time-consuming and requires detailed knowledge of the system.

Overall conclusions and implications of the Task 5 modelling exercise

The Task 5 modelling exercise represented a coordinated attempt to integrate hydrogeochemistry with hydrogeology in the light of future repository site characterisations and performance assessment requirements.

General conclusions

- Groundwater mixing ratio simulations based on M3 calculations provided a convenient means to integrate hydrogeochemistry and hydrogeology.
- The simulations showed that the results over the time period simulated (about 5 years) were sensitive to the boundary conditions of the ‘regional model’ with dimensions of approximately 2 x 2 x 1km (last figure is depth). Simulations indicated that the transport times from the vertical boundaries were possibly shorter than the simulation time, thus having a greater impact on the simulated chemical composition of the inflowing water to the tunnel at the control points.
- The reliability of the given boundary conditions was an issue discussed at length, especially the western boundary, since it was mainly based on one deep borehole.
- Another issue addressed was whether the hydrogeochemical data represented conditions in the entire rock mass or mainly the most conductive features, i.e. the issue of how to interpolate in a reasonable way to obtain initial and boundary conditions solely for the Hydraulic Conductor Domains and Hydraulic Rock Mass Domains.
- Below the Baltic sea the shortest transport times from the boundaries (sea bottom) was in the scale of approximately one month, indicating that the sampling programme carried out was inadequate to record the rapid dynamics of the system during tunnel construction.
- In some cases a full and direct comparison between modelling groups was not possible due to different levels of ambition, achievement, available time and resources and model development.

Understanding the Äspö Site

What additional insight has Task 5 provided in further understanding the dynamics and evolution of the groundwater flow system at Äspö?

The provided major hydraulic features (Hydraulic Conductor Domains), with one exception, appear to have been relevant and consistent concerning hydraulic responses. The responses from the inflow to the shafts indicated the presence of a previously unknown, fairly transmissive feature intersecting, or hydraulically well connected to, the shafts.

Was hydrogeochemistry successfully integrated in the hydrodynamic modelling exercises? What is the future of hydrogeochemical integration?

The modelling integration of hydrogeochemistry and hydrogeology has been largely successful given the time and resources made available; the following points can be emphasised:

- A common approach was to derive a calibrated hydrodynamic model based on hydrogeology. This model was then used to predict the chemical distributions and then recalibrated in some but not all cases to the measured chemical values by varying the fracture properties and boundary conditions.
- In some of the modelling carried out the travel velocity was poorly predicted. The hydrogeochemical data provided the opportunity to refine these velocities.
- The use of hydrogeochemical data was required to calibrate the hydrogeological model and also the aperture and storage parameters.
- Geochemical reaction modelling was used to quantify the influence of reactions on the groundwater chemistry during mixing; this can be used as a means to exclude locations were reactions dominate, so that only locations characterised by mixing are hydrodynamically modelled (e.g. using complex coupled reaction models).
- Confidence in a reliable hydrogeochemical conceptual model is another critical factor when initially deciding the boundary conditions to hydrodynamically model the system.
- The future direction of hydrogeochemical integration should include further refinement of its use as demonstrated in the Task 5 modelling approach, for example:

    - helping to constrain initial and boundary conditions
    - providing reference water mixing proportions for time-series samples collected at hydraulically strategic localities

Site characterisation implications

What experience/knowledge gained from Task 5 can be successfully transferred to the site characterisation programme?

Several important implications from the Task 5 exercise are relevant to site characterisations:

- Important to have a sampling strategy in the regional scale to collect data for the definition of initial and boundary conditions with reasonable resolution.

- Important to judge what can be considered as a large scale model (regional model?) to test a geoscientific model description in a similar way as Task 5. This has implications to define initial conditions at the site and regional scales.

- Important to have a sampling strategy during repository construction to collect data for the definition of the transient conditions with a reasonable resolution.

Repository Performance Assessment (PA) implications

What experience/knowledge gained from Task 5 can be successfully transferred to repository performance assessment issues?

Although the modelling groups were not expected to discuss their results with reference to performance assessment (PA) implications, such a general discussion was implicit in the Task 5 rationale and has therefore been addressed.

A key requirement for a repository performance assessment (PA) is a description of radionuclide release and transport from a leaking defective canister in the near-field, into the geosphere and eventually to the biosphere. This description is based on sound geoscientific knowledge of the various disciplines (i.e. geology, rock mechanics, rock thermal properties, hydrogeology, hydrogeochemistry and the transport properties of the geosphere, and also the surface ecosystems) which provides an important basis for determining the overall confidence in the system or site in question. However, maximum confidence, reliability and justification can only be obtained by integrating/coupling these disciplines and judging their consistency. To some extent geology and rock mechanics are intrinsically coupled, and to a certain extent also geology and hydrogeology. What Task 5 has attempted to address is the potential to integrate hydrogeology with hydrogeochemistry and to assess the implications of this exercise to repository performance assessment.

Groundwater flow models at various scales are an important part of constructing the geosphere model(s); from a hydrodynamic viewpoint this will involve numerical modelling at the regional, local and block site scales. In addition, and equally important to knowing the present-day groundwater flow situation, is understanding the long-term hydraulic and hydrogeochemical evolution of groundwater systems as a basis of predicting future repository conditions. For example, modification of topography caused by erosion and the influence of glacial events (e.g. permafrost) will cause complex hydrodynamic changes. It is in this area that the integration of hydrogeochemical information, in terms of interpreting the palaeohydrogeology, plays a key role in predicting and modelling long-term hydrodynamic stability at potential repository sites.

Task 5 can be described as a 'large' Local Scale Model (i.e. repository scale) exercise. The question is whether Task 5 during the past four years has made any significant progress in integrating hydrogeochemistry in PA-related hydrodynamic models? Although the areas of mathematical integration are limited, several useful accomplishments have been forthcoming:

- Simple simulation of mixing ratios was used a basis to calibrate (e.g. consistency check) the hydrogeological model.
- Hydrogeochemical time-series data at the selected control points reflected changes in the hydrodynamic flow conditions and were useful therefore for calibration purposes.
- Use of salinity (density) data to simulate large-scale hydrodynamic flow conditions was considered essential by some groups.
- Coupled flow and multicomponent reactive transport modelling was carried out by two groups; this was identified as an area for further development.
- Modelling and integration strategies were to some extent discussed and described.

In terms of direct application of Task 5 models to a PA model chain of the type used in the SKB SR-97 safety case, it is not valid. However, Task 5 has provided examples of some modelling exercises that could be transferred to PA for use in consistency checks and confidence building to show that the geosphere is reasonably well described.

As a general conclusion, the use of hydrogeochemistry in safety and performance assessment was considered relevant to: a) the development of site-descriptive (and conceptual) models at all scales, b) independent, consistency checks, and c) predict hydrogeochemical conditions at repository depths over repository timescales. Future progress should involve the continued development of coupled flow and reactive transport models which can improve the integration and testing of PA-related models, and also more use of hydrogeochemical transient scenarios.

Concluding comment

Even though the extent of mathematically integrating hydrogeochemistry with hydrogeology within Task 5 appears to have been limited, considerable progress has been made in other areas of importance. For example, Task 5 has provided the opportunity to bring together two scientific disciplines which traditionally have tended to work in parallel rather in close collaboration. This is an important first step. The process of understanding, interacting and integrating has now been initiated and, given more time and resources, the degree of scientific integration and model development would have been greater. In any case, there is now a much stronger appreciation that the use of hydrogeochemistry can lead to an increased understanding of hydrogeology, and *vice-versa*.

Contents

Appendices

1 Background

1.1 Äspö Hard Rock Laboratory

In order to prepare for the localisation of a suitable site and licencing of a spent fuel repository SKB has constructed an underground research laboratory, the Äspö Hard Rock Laboratory (HRL). Construction commenced in the autumn of 1990 near Oskarshamn in the southeastern part of Sweden (*Fig. 1-1*). The laboratory was completed in 1995 and consists of a 3.6 km long tunnel excavated in crystalline rock down to a depth of approximately 460 m (*Fig. 1-2*).

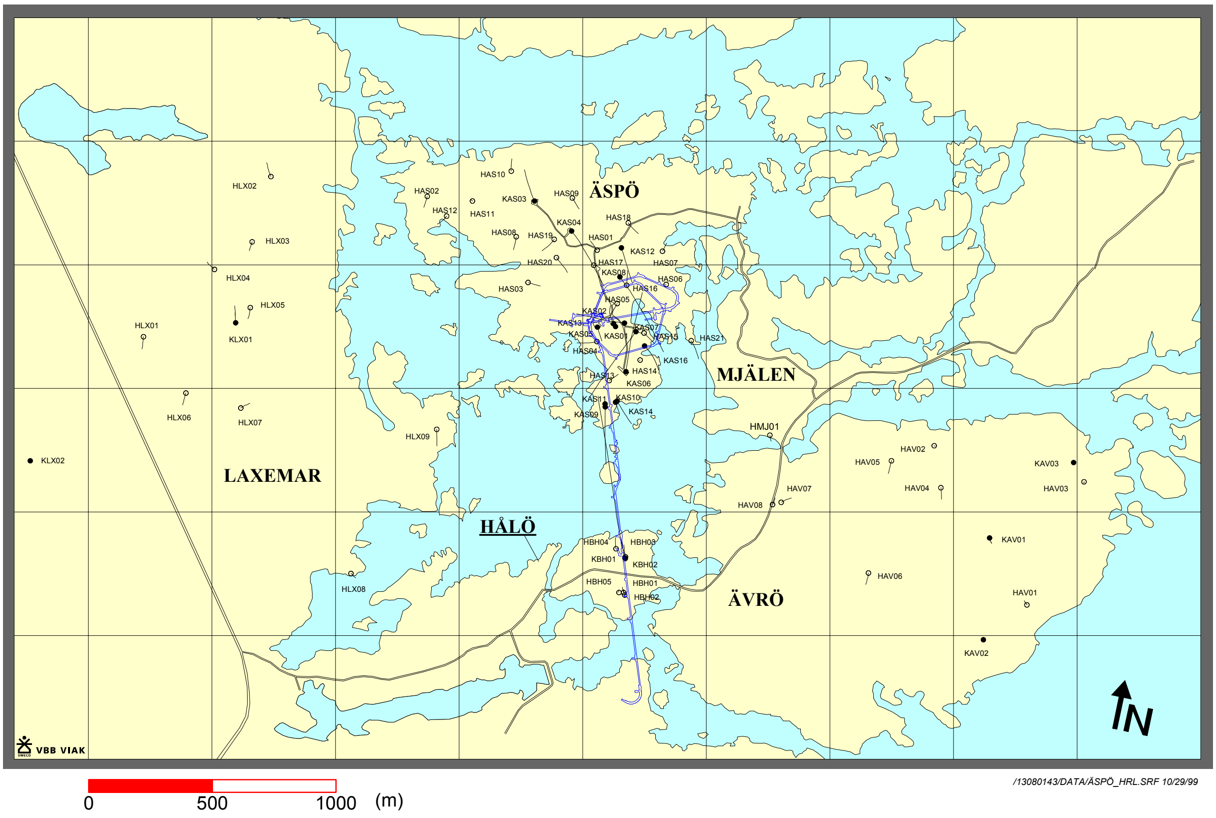


***Figure 1-1.** Location of the Äspö Hard Rock Laboratory (HRL)*

Prior to, during and subsequent to completion, research concerning the deep geological disposal of nuclear waste in crystalline rock has been carried out. Central to this research has been the characterisation of the groundwater flow system and the chemistry of the groundwaters at Äspö prior to excavation (Pre-investigation Phase) and subsequently to monitor changes in these parameters during the evolution of laboratory construction (Construction Phase). There is, therefore, a considerable amount of available data for modelling purposes compiled over a 15 years period. To successfully understand and model the groundwater flow and hydrogeochemistry of a potential radioactive waste site is important

Figure 1-2. *Overview of the Äspö HRL tunnel. The maximum depth of Äspö HRL is 460 m below the ground surface. The vertical lines show the elevator and ventilation shafts from the ground surface.*

since these two processes will play a central role in determining potential radionuclide transport pathways from the repository to the biosphere in the event of leakage from one or more defect canisters. The Äspö HRL site provides an excellent opportunity to test and develop suitable models for the purpose of assessing the long-term performance of a deep geological repository for radioactive wastes in crystalline rock.

1.2 Task 5: Purpose and aim

Traditionally, hydrogeology and hydrochemistry have been treated separately in site characterisation investigations and this is partly reflected in the lack of mathematical models and codes to integrate or couple successfully the two disciplines. This is unfortunate since knowledge of the groundwater flow and hydrochemistry is important for the long-term safety and performance assessment of a repository. To integrate the two disciplines should give greater confidence in describing present conditions, past conditions (palaeohydrogeology) and consequently predicting future conditions. Of course, successful integration depends on understanding the mechanisms and the processes controlling the geochemical evolution and dynamics of the groundwater system.

Groundwater flow models are used to describe the flow cycle where recharging groundwater is slowly transported down through the deep geologic formation (geosphere) and then back to the vicinity of the geosphere/biosphere interface where it eventually discharges into the biosphere. The distribution of the flow at the repository level and the transport time from the repository to the biosphere are critical for the assessment of possible nuclide migration from a defect waste canister. In addition, the chemical composition of the groundwater is also important since it will largely influence the dissolution rates, concentrations and retardation of hazardous radionuclides (e.g. Pu, Np, Tc etc.). The composition and evolution of the groundwater chemistry is a result of mixing and water/rock reactions along the groundwater transport pathways. Therefore, integration of hydrodynamics and groundwater chemistry is essential to gain confidence in the solute transport models employed in performance assessment. However, there are several conditions that make this integration problematic.

There are basic differences in application. For example, hydrogeochemical information is used to understand the groundwater origin and evolution, while hydrogeological models generally simulate the present day hydrodynamic conditions. Moreover, groundwater flow models are usually based on simulations of the present day conditions, while the hydrogeochemistry is resulting from several events that are different from the present day situation. The key to a successful integration of hydrological and hydrogeochemical models must therefore be to understand the mechanisms and processes controlling the evolution and dynamics of the groundwater system.

In a site with a complex groundwater history such as Äspö, the different conservative natural water tracers may each have several sources, which means that a single natural tracer cannot be used for tracing the origin/evolution of the water flow; for example, an old sea water may be displaced by a modern sea water without affecting the salinity. In a transient groundwater system the chemical changes may take much longer than the time indicated by conducting fracture tracer tests using conservative species; the transport time of a dissolved species is faster than the changes in the entire chemical system. Furthermore, the parts of the system that have low permeability may be in a transient state, rather than a steady state, in response to changes over the last few thousands of years. This applies in particular to the chemical composition of groundwater that takes a longer time to respond to changes along the flow paths than to changes in hydraulic pressure.

At this juncture it is also important to recognise that tunnel construction at Äspö has resulted in a very transient system caused by a massive groundwater drawdown which differs significantly, both hydraulically and hydrochemically, from a natural (or undisturbed) system or even a pump-test. In such a transient system the time scale for a specific response varies considerably depending on individual processes. Pressure responses will tend to be fast, advective travel times may be rather slow and salinity changes, for example, may be very slow because of diffusion processes and density-dependent flow into or out of stagnant zones.

There is a need to integrate hydrodynamics with hydrogeochemistry. Some attempts have been made in the past, for example, a comparison and calibration of hydrogeological and hydrogeochemical models have been described by *Vomvoris (1996).* In the Äspö context *Löfman and Taivassalo (1995)* simulated the salinity and pressure fields around Äspö island. However examples are few and integrating these two disciplines still remains an area of limited experience in site characterisation investigations. Consequently, Task 5 (Impact of the tunnel construction on the groundwater system at Äspö. A hydrological-hydrochemical model assessment exercise) was initiated to test, develop and integrate different modelling approaches to achieve a more realistic simulation of the groundwater flow systems at Äspö. Of course models to simulate the hydrodynamics of groundwater flow systems have been long available, but the mathematical coupling of hydrogeochemistry has been restricted. The most appropriate data have related mainly to physical parameters such as groundwater salinity/density that can be readily integrated mathematically.

The major aim of Task 5 was to ultimately integrate hydrochemistry and hydrogeology. The proposed Task 5 modelling was also expected to be useful for confidence building, i.e. development and testing of models for predictive purposes. For example, predicting that any hydrodynamic transient changes (e.g. during glaciation) would still ensure that the groundwater chemistry (i.e. redox) remains within acceptable safety limits. This modelling approach could then be used for any future repository site investigations, especially in a crystalline bedrock environment.

The specific objectives were:

- To assess the consistency of groundwater flow models and hydogeochemical mixing-reaction models through integration and comparison of hydraulic and hydrogeochemical data obtained before and during tunnel construction, and
- To develop a procedure for integration of hydrological and hydrogeochemical information which could be used for disposal site assessments.

Task 5, described in *Wikberg (1998),* commenced in 1998 and was finalised in 2002. Participating modelling teams in the project represent ANDRA (France; three modelling teams – ANTEA, ITASCA, CEA), BMWi/BGR (Germany), ENRESA (Spain), JNC (Japan), CRIEPI (Japan), Posiva (Finland), and SKB (Sweden; two modelling teams – CFE and Intera (now GeoPoint)). Funding organisations:

Svensk Kärnbränslehantering AB (SKB), Sweden,
Power Reactor & Nuclear Fuel Development Corporation (JNC), Japan
Central Research Institute of Electric Power Industry (CRIEPI) Japan
Agence National Pour la Gestion des Déchets Radioactifs (ANDRA), France
POSIVA Oy, Finland
Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie (BMW), Germany
Empresa Nacional de Residuos Radiactivas (ENRESA), Spain

1.3 The summary report

This report summarises the main approach, execution and conclusions of Task 5 related to modelling the hydrodynamics and hydrogeochemistry to describe the groundwater changes incurred during the construction of the Äspö tunnel. Under the auspices of the Äspö HRL International Task Force, parallel modelling efforts by groups using different approaches have been carried out. An immense amount of data has been generated by the modelling exercise and this report has been structured to provide the reader with adequate selected material to appreciate the overall nature of the data obtained, the modelling efforts conducted, and the main conclusions reached. Furthermore, this summary report provides a starting point for the External Review Report (*Bath and Jackson, 2002*) that will focus on an objective evaluation of Task 5. The purpose of this Review Report is to assess the success or otherwise of Task 5 in achieving the specified objectives, to indicate the remaining areas of weakness, and to provide guidelines as to where future emphasis should be placed to improve the results.

Chapter 2 of this Summary Report briefly introduces the geological and hydrogeological setting at the Äspö site and Chapter 3 outlines the sources of hydrogeological and hydrochemical data used in the Task 5 modelling exercises. These include data from the 'Pre-investigation Stage' and the 'Tunnel Construction Stage' representing the undisturbed and disturbed groundwater conditions respectively. Chapter 4 presents the background perspectives to the Task 5 modelling, the different model-types available, introduces the scope, objectives and rationale behind the Task 5 modelling, a description of the model construction and the approaches used by the modelling groups and, finally, the various means of integrating hydrogeochemistry and hydrogeology. This is followed by a summary and discussion which compares the broad similarities and differences in the modelling approaches and how these differences may influence the modelled results. Chapter 5 is devoted to the application and use of the Äspö data and the modelling results. Also included is a discussion and conclusion section where unresolved issues are addressed. Chapter 6 presents the overall conclusions; in addition to a summary of the Task 5 modelling, this chapter also addresses how Task 5 has helped to further understand the Äspö site, the implications for site characterisation in general, and the implications for repository performance assessment. The appendices include a data and documentation overview, executive summaries of all the modelling work reported and a modelling evaluation Questionnaire.

2 Geological and hydrogeological setting

The island of Äspö comprises a slightly undulating topography of well exposed rock with a maximum elevation of about 14 m, characterised by small drainage basins with some peatlands and sediments in the topographic lows. There are no perennial streams on the island, the surface water being drained to the Baltic Sea by the peatlands, sediments or directly to the sea. West of Äspö island, on the Laxemar mainland area, discharge areas are along the coast and also in peatlands and along small streams flowing towards the Baltic sea. The annual mean precipitation and temperature of the area are about 550 mm/year, and 6.5°C respectively, with the annual sea level fluctuations generally within ± 0.5 m. The groundwater table elevation above the mean sea level is about 30% of the elevation of the topography above mean sea level, within a few hundred metres from the coastline.

The geology (*Fig. 2-1*) is characterised by a red to grey porphyritic granite-granodiorite of Småland type, containing microcline megacrysts up to 1 to 3 cm in size. To the south of the island a redder granite variety, the Ävrö 'true' granite, outcrops, containing small (<1 cm) sparsely distributed microcline megacrysts. Within the granite are east-west trending lenses/sheets of fine-grained granite and also greenstone (metabasalt) which are usually strongly altered. Subordinate lenses of fine-grained grey metavolcanites (of dacitic

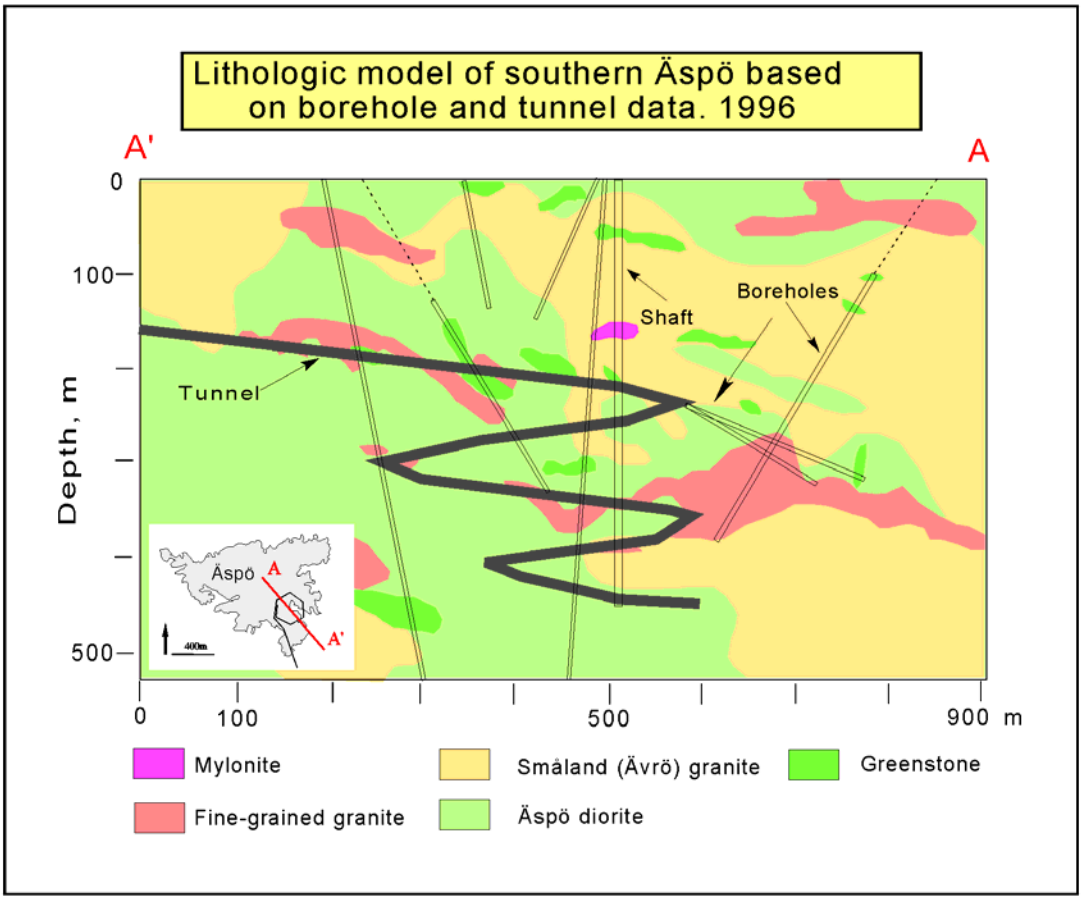


Figure 2-1. *Southern Äspö, schematic illustration of the lithology (Rhén et al., 1997a)*

composition) also occur. Both of these rock types predate the Småland granite. Finally, small occurrences of pegmatite commonly occur as very narrow dykes (decimetres in width). Structurally (*Fig. 2-2*), Äspö island is divided into two main blocks by a NE-trending regional shear zone (EW-1); this reflects the main structural anistropy of the island which is parallel to an almost vertical, more or less penetrating foliation trending NE-ENE. In both blocks the Småland granite, with associated greenstones and fine-grained granite/aplite varieties, dominates, although in the southern block below 300 m, more basic dioritic varieties of the Småland granite (i.e. Äspö diorite) begin to dominate.

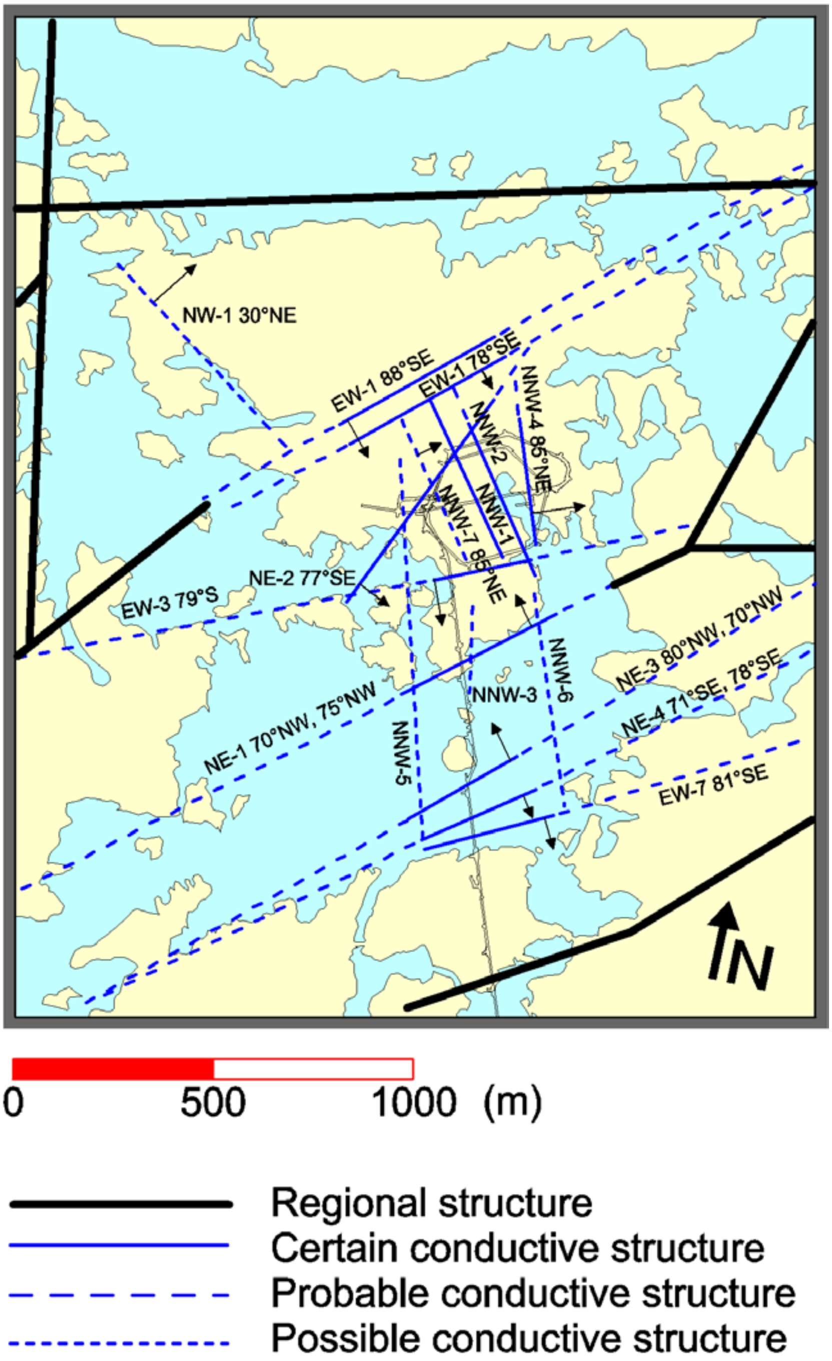


Figure 2-2. *Major structural subdivisions and hydraulic conductors of Äspö island and its vicinity (Rhén et al., 1997a)*

The EW-1 shear zone, which is vertical to subvertical to the north, consists of strongly foliated heterogeneous Småland granite containing a large number of mylonitic lenses and greenstone xenoliths. Highly fractured zones (5-10 m wide), alternating with more normally fractured rock, complicate the shear structure that has also undergone substantial weathering, seen as oxidation of magnetite to haematite and Fe-oxyhydroxides. This explains the negative aeromagnetic anomaly that is observed.

The northern block is more fractured than its southern counterpart; in both cases the fractures are vertical to sub-vertical in orientation.

The main fracture filling mineral phases consist of, in decreasing order of frequency: group A (chlorite, calcite), group B (haematite, Fe-oxyhydroxides, epidote, fluorite), and group C (pyrite, magnetite, laumonite/prehnite, gypsum).

The areal distribution of hydraulic conductivity at Äspö on the site scale is heterogeneous. Generally the fine-grained granite/aplite tends to be the most conductive unit, probably because it is the most competent rock type and is therefore inclined to fracture easily in response to tectonic movement. The increased fracture frequency in the northern block of Äspö reflects a correspondingly higher hydraulic conductivity. Furthermore, there is also a general decrease in the variability of hydraulic conductivity with depth.

Recharge/discharge and groundwater flow through Äspö is controlled by the major tectonic fractures and discontinuities with a general groundwater flow trend, at least in the upper 500 m or so, from north to south towards the NE-1 zone, facilitated by the NNW-trending vertical to subvertical fractures (Fig. 2-2). The major E-W trending shear zone (EW-1) is a strong recharge feature. Following tunnel construction the main groundwater flow is from the south, but the drawdown of meteoric water from shallower levels, in addition to minor inputs from the north via EW-1 and the NNW-trending fractures, also occurs towards the tunnel.

3 Available sources of data

3.1 General

The construction of an underground laboratory some 460 m below the island of Äspö forms part of the overall SKB strategy to test, not only the construction techniques for deep repository excavation, but also the various methods and protocols required to obtain a three-dimensional model of the geology and groundwater flow and chemistry within a fractured crystalline bedrock similar to that envisaged for the final disposal of spent nuclear fuel. Äspö was chosen because it geologically represents a variety of crystalline bedrock environments typical for the Fennoscandian Shield. To demonstrate and quantify many of the site-dependent parameters that will ultimately control the safety of a final repository (e.g. geology, hydrodynamics and hydrogeochemistry), together with evaluating the functions of the various engineered barrier systems in a realistic environment, should go a long way in an overall performance assessment analysis.

Investigations at the Äspö HRL fall into three categories: 1) Pre-investigation Phase (1986-1990), 2) Construction Phase (1990-1995), and 3) Operation Phase (1995-2050?). The results from the pre-investigation and construction phases have been presented in a large number of Progress Reports, International Cooperation Reports, Technical Reports and also in the open scientific literature. The feasibility and usefulness of site investigation methods in general are described in *Almén et al. (1994).* An overview of the specific investigation methods used during 1986-1995 is presented in *Stanfors et al. (1997a),* summary of results in *Rhén et al (1997b)* and a detailed evaluation of results is presented in *Stanfors et al. (1997b)* and *Rhén et al. (1997c).* Updated models of Äspö based on site characterisation data obtained during 1986-1995 are reported in *Rhén et al. (1997c).*

With the completion of the pre-investigation and construction phases a major milestone was reached, namely an assessment of the reliability of site characterisation methods. This aspect of site characterisation is important since the results from the investigations will be used:

- to show whether a site has suitable geological properties for a deep repository,
- to provide data and knowledge concerning the host bedrock so that a preliminary emplacement of the repository in a suitable rock volume can be carried out to provide a basis to analyse the feasibility of construction,
- to provide the necessary data for a preliminary safety assessment which, in Sweden, shall serve as support for an application under the Management of Natural Resources Act (NRL) and the Nuclear Activity Act (KTL) to carry out detailed site characterisation, and
- to provide data for the planning of a detailed site characterisation that will take place during excavation from the bedrock surface down to repository levels.

The Task 5 modelling exercise centres on data accumulated during the pre-investigation and construction phases.

3.2 Pre-investigation phase

3.2.1 General

The Pre-investigation Phase, extending from the surface to around 1000 m, was aimed at siting the laboratory, describing the natural hydrogeological, hydrochemical and geochemical conditions in the bedrock, and predicting the changes that will occur during the excavation and construction of the underground laboratory. This phase was extremely important in that it provided the only opportunity to study the natural, ‘undisturbed’ groundwater conditions in the bedrock.; in particular to provide a reliable reference point for all subsequent hydrogeological and hydrogeochemical investigations carried out during the construction and operation phases. Without such reference data, interpretation of subsequent hydraulic and hydrochemical changes would only reveal trends that were active over a particular period of time. Without these primary data to constrain the boundary conditions it would be impossible to test and describe the main processes of interest.

Specifically, the pre-investigation site studies for the Äspö HRL were planned to meet two requirements:

- to test the ability to obtain a thorough understanding of the rock conditions based on surface investigations including the use of boreholes drilled from the surface, and

- to conduct investigations necessary to design the underground facility so that it could be constructed with presently available technology, without major problems, down to a depth of 500 metres. The facility should also be designed to meet the needs for research, development and demonstration studies in the operation phase.

3.2.2 Geology and tectonics

During the pre-investigation phase a number of methods were tested and used to develop suitable site-specific geostructural models; an example is reproduced in *Figure 3-1.* To address the regional scale geology, airborne geophysical measurements (magnetic, electromagnetic and radiometric) together with lineament interpretation of terrain models were used to identify the major fracture zones and the general lithology. By means of surface mapping, petrophysical measurements of rock samples and ground geophysics (gravity, refraction seismics, etc), different types of geophysical anomalies were identified and the indicated fracture zones characterised.

On a site-specific scale, an extensive drilling programme including measurements in the boreholes was carried out. Downhole geophysics and radar were systematically utilised; TV logging, televiewer and Vertical Seismic Profiling were conducted in a few boreholes. Detailed geophysical ground surface measurements were performed, including VLF, resistivity, magnetic, radiometric, seismic refraction and reflection (limited use), and integrated with detailed geological mapping of the surface bedrock.

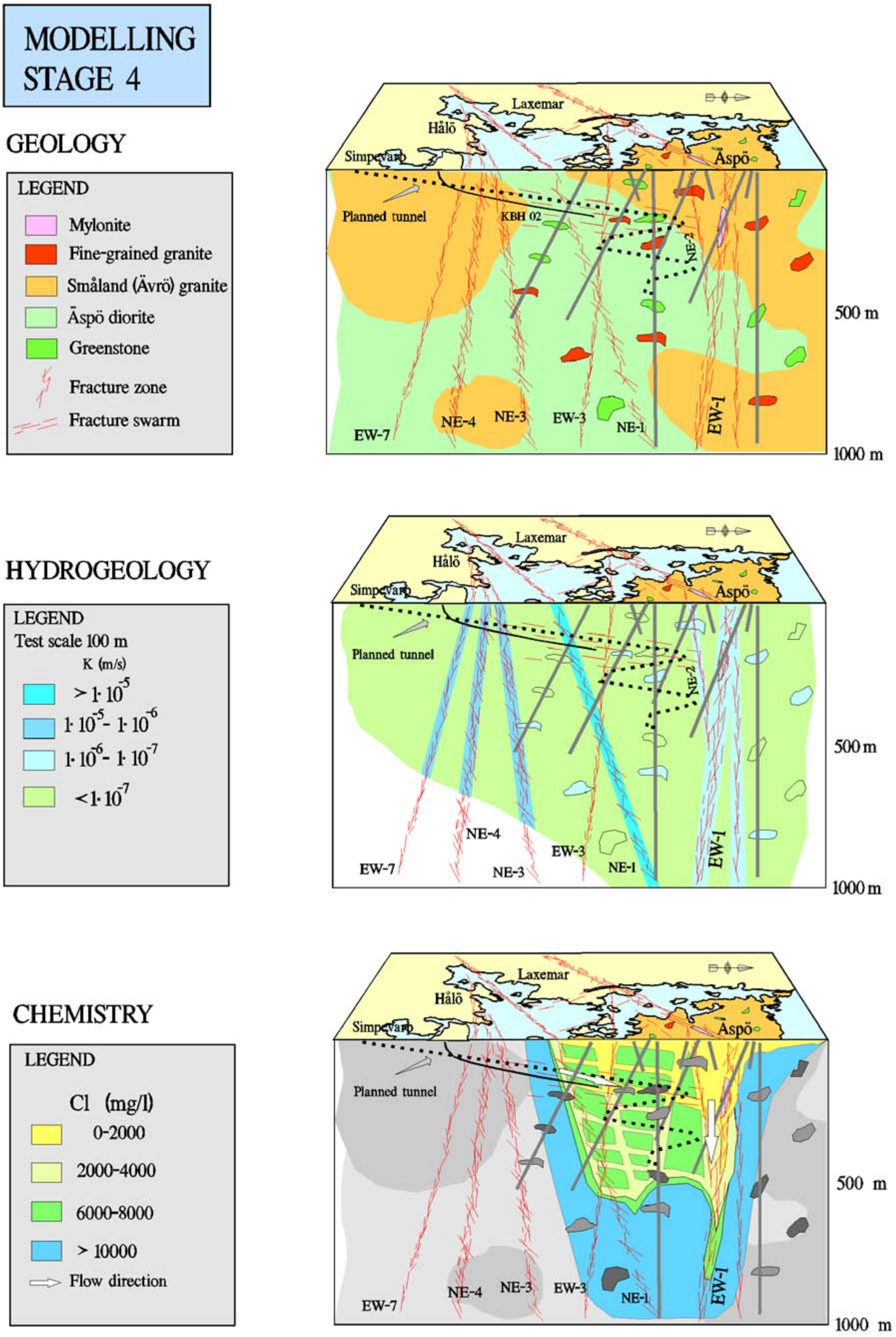


Figure 3-1. *Stage 4 in the model evolution of the Äspö site. Note the attempt in the chemical model to introduce the reality of a fracture-controlled groundwater flow system and the corresponding variations in groundwater chemistry (Rhén et al., 1997a).*

These investigations confirmed at depth the major sub-vertical fractures NE-1, NE-2, NE-3, NE-4, EW-3 and EW-7 (*Fig. 3-1*). Not shown on the figure are discontinuous, a few sub-horizontal fracture swarms and two minor fracture zones in the tunnel. In combination with hydraulic testing a NNW-system of minor sub-vertical fractures was indicated and thought to connect the major water-bearing NE-trending fracture zones.

3.2.3 Hydrogeology

A number of pre-investigation methods were used to determine the hydrogeological model. The hydraulic properties of the hydraulic conductor domains (HCDs) and the hydraulic rockmass domains (HRDs) located between the HCDs were characterised by a number of different hydraulic tests:

- airlift pumping or submersible pumping of percussion drilled boreholes and 100 m sections of core-drilled boreholes,
- pump testing and cleaning of borehole (performed directly after drilling),
- flow-meter logging,
- injection tests (packer spacing 3 or 30 m),
- interference tests,
- dilution tests,
- monitoring of water pressure in the rock-mass,
- long-term monitoring was also performed.

The hydrogeological description of the rock was derived from integrating the evaluated hydraulic parameters with the geological model (*Fig. 3-1*). The first three methods were performed more or less systematically in all cored boreholes. The percussion-drilled boreholes were either tested by airlift pumping or using a submersible pump. About 100 pumping tests were performed with test sections exceeding 100 m. Injection tests with a packer spacing of 3 m (about 1200 tests, injection and recovery periods about 10 + 10 minutes) were performed in 8 cored boreholes and injection tests with a packer spacing of 30 m (65 tests, injection and recovery periods about 2 h + 2 h) were conducted in 3 cored boreholes. Roughly 20 interference tests were performed, generally with a pumping period of 3 days and a pressure recovery period of 2 days. Two sustained interference tests were also performed, with pumping periods of about 60 and 30 days but with somewhat shorter recovery periods.

Several important hydraulic features were identified striking approximately NW, ENE, NE and NNW. Furthermore a total of five different rockmass domains were identified. Two of them, the ‘Northern Äspö’ block and the ‘Äspö Shear Zone’ confirmed earlier estimations, however the ‘Southern Äspö’ block is now considered to constitute two blocks. A rather narrow range of probable transmissivity was assigned to each hydraulic conductor domain and included in the model as a deterministic feature. The transmissivity was mainly based on the test results but in a few cases a value was assigned based on expert judgement in the absence of measured data. Data from the injection tests, with a packer spacing of 3 m, were analysed statistically to provide estimates of the hydraulic properties of the hydraulic rock mass domains (*Fig. 3-1*).

3.2.4 Hydrogeochemistry

In the pre-investigation phase, on a semi-regional scale, data were obtained from shallow, 100 m deep, percussion-drilled boreholes at Äspö; nearby mainland sites at Laxemar and Ävrö were also investgated. Site-scale investigations included samples from sections isolated by packers in the deep core-drilled boreholes on Äspö and complemented by two deep boreholes at Laxemar. Most of the sampling at Äspö was done in the first three cored boreholes (KAS01-KAS03) which penetrated the northern and southern parts of the island and intersected the Äspö EW-1 shear zone.

On the average there is a linear increase in salinity with depth, with an increase of 1000 mg/L for each 100 m. However, despite the linear increase in salinity, different water types can be distinguished. Glacial meltwater can be identified due to its very low $\delta^{18}O$ value, and modern and old Baltic Sea water and meteoric freshwater are also distinguished on the basis of their ratios of major components. At depths of more than 500 m at Äspö island the water is not affected by the different stages of the Baltic Sea evolution that have taken place since the last glaciation some 10 000 years ago.

The sampled groundwater is in general reducing at depths exceeding a few tens of metres. However, in exceptional cases, which are fracture-specific, oxidising conditions may prevail down to 100 m due to localised hydraulic gradients. Oxygen-rich surface water rapidly becomes anoxic as it percolates into the rock due to microbial activity and also due to the natural buffering capacity of fracture minerals rich in ferrous iron (e.g. biotite/chlorite).

It was found that bacteria are important for establishing high concentrations of dissolved iron and bicarbonate and that bacterial reduction of Iron (III) minerals and sulphate increase the reducing capacity of the groundwater.

Based on observed changes in groundwater chemistry and hydraulic conditions with depth, *Laaksoharju and Nilsson (1989)* produced generalised models of the Äspö site. A more detailed hydrogeochemical evaluation of the site was subsequently carried out by *Smellie and Laaksoharju (1992)* where interpretation was closely integrated with the geological and hydrogeological observations. In this case the quality of the groundwater was initially classified as being representative or not; suitable chemical, isotopic and mineralogical data were used then to derive the hydrogeochemical evolution and origin of the groundwaters. Finally, a conceptual groundwater flow model was constructed based mainly on borehole geochemical trends and detailed observations from individual borehole sections (Fig. 3-1).

In addition to establishing and modelling present-day groundwater conditions, the ‘undisturbed’ bedrock and groundwater environments allow the possibility of reconstructing the palaeo-evolution of the site. Providing some insight into the effects of the last glaciation(s) may establish a basis for predicting groundwater conditions under future glacial conditions. As a result, the various stages of the Baltic Sea evolution, particularly since the last glaciation some 10 000 years ago (Fig. 3-2), have been conceptualised as part of the pre-investigation phase studies *(Smellie and Laaksoharju, 1992; Laaksoharju et al., 1999).*

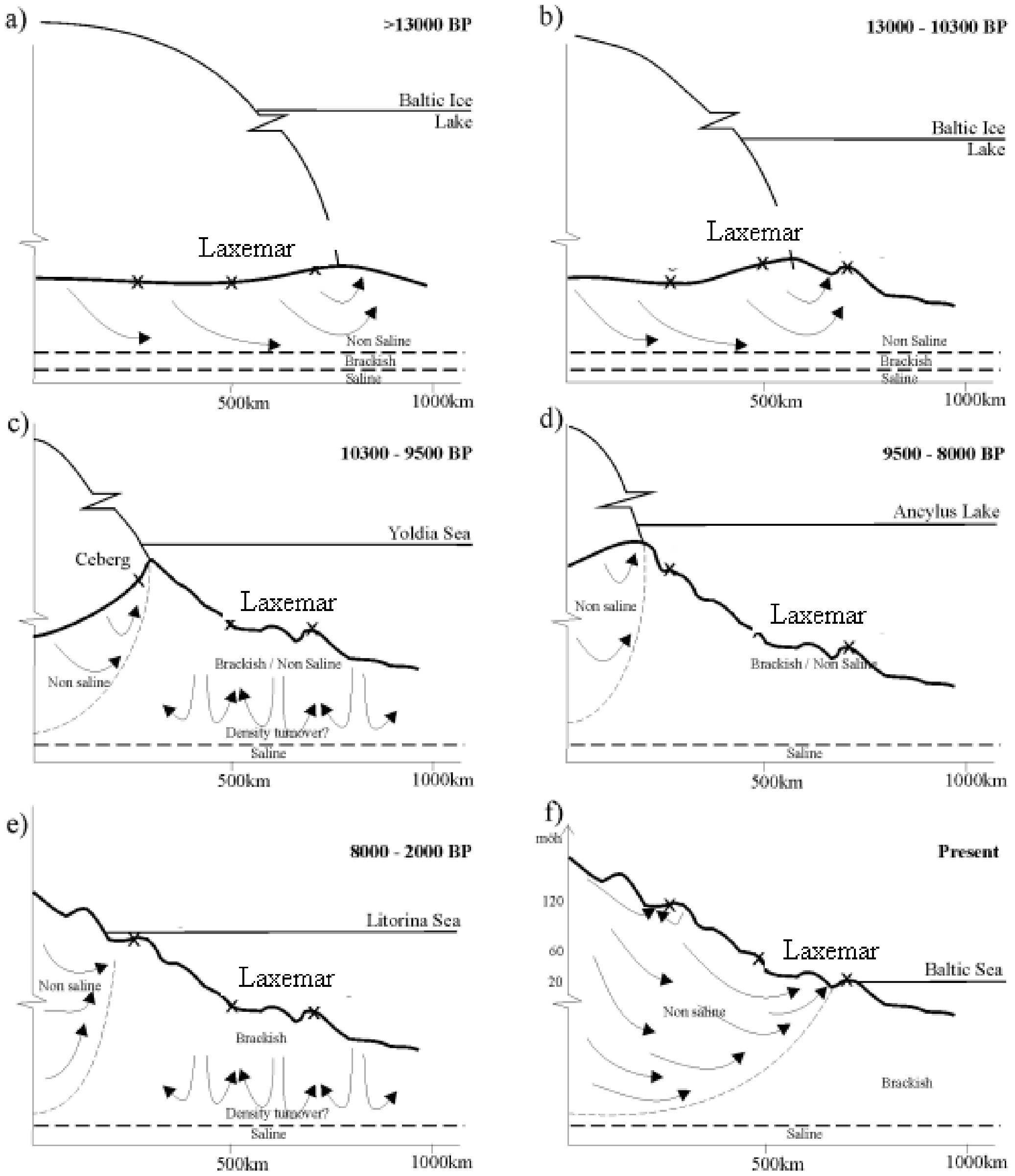


Figure 3-2. *Conceptual post-glacial scenario along an E-W section at the Äspö site and the adjacent Laxemar mainland. Possible flow lines, density driven turnover, non-saline water interfaces are shown: a) Injection stage of glacial meltwater into the basement, b) Baltic Ice Lake stage, c) Yoldia Sea stage, d) Ancylus Lake stage, e) Litorina Sea stage, and f) present-day stage (after Laaksoharju et al., 1999).*

3.2.5 Groundwater-flow conceptual model: 'Undisturbed' conditions

Comparing and integrating the three conceptual models resulting from Model Stage 4 (*Fig. 3-1*), it is possible to infer, at least qualitatively, the major directions of the groundwater-flow paths and also emphasise the heterogeneous distribution of the groundwater chemistry and hydraulic properties within the Äspö bedrock at different scales. In *Figure 3-3* the 'undisturbed' conditions have been conceptualised in greater detail in terms of groundwater chemistry and residence times. In addition, a more realistic representation is given of the major hydraulic features and the nature of matrix fluid/groundwater at the cm scale.

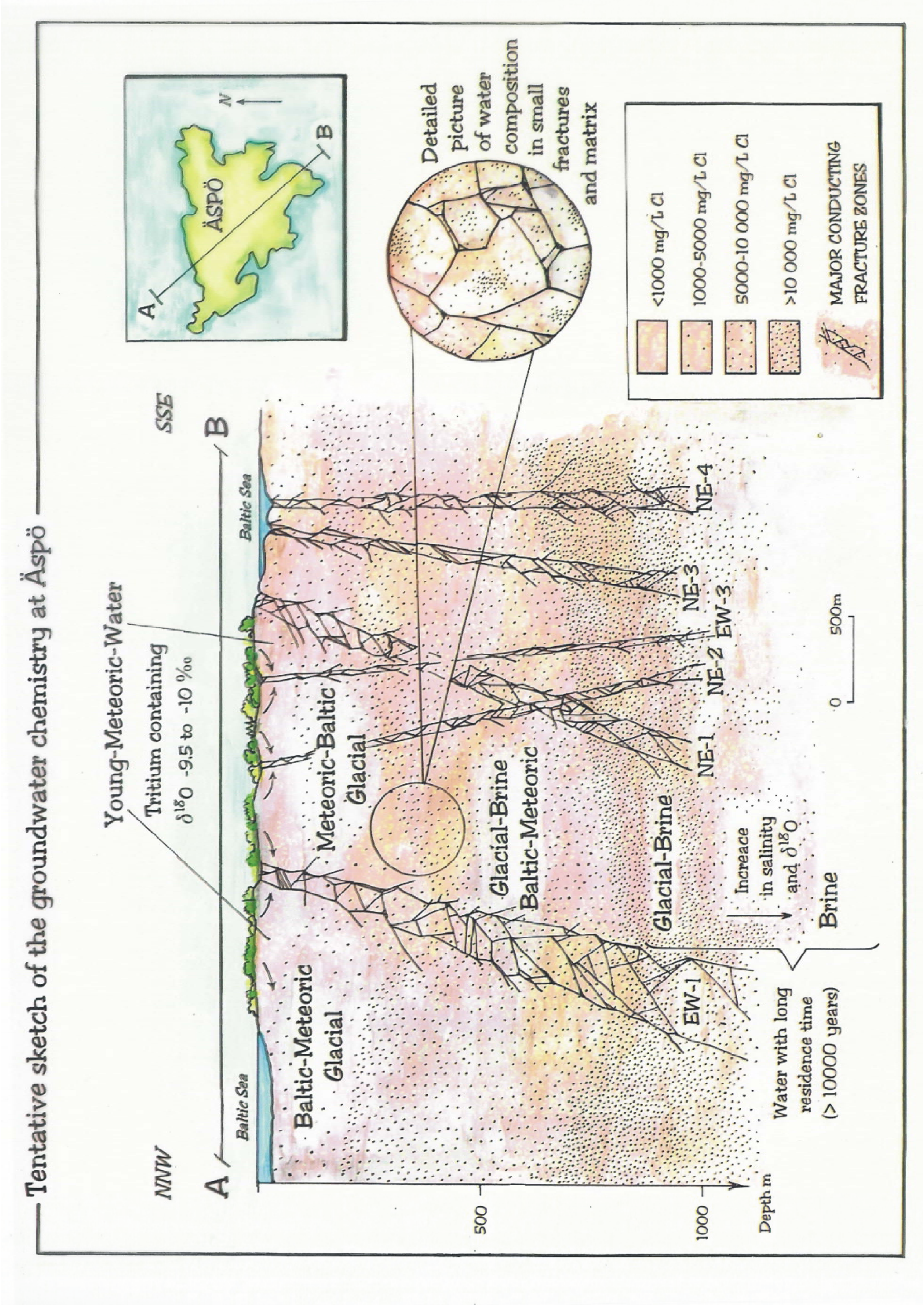


Figure 3-3. *Conceptual model of the'undisturbed' groundwater chemistry at Äspö. From Tullborg, E-L. in Bath et al. (2000), based on Smellie and Laaksoharju (1992).*

3.3 Construction phase

3.3.1 General

Following the pre-investigation phase, construction of the access tunnel and underground facilities ('Construction Phase') commenced in 1990 with completion in 1995. The maximum depth of the laboratory is 460 m and the tunnel has a total length of 3 600 m (*Figs. 1-1, 1-2*). During this phase extensive investigations, tests and experiments were carried out in parallel with the excavations. The focus of the experimental work was mainly to check the reliability of interpretations based on the pre-investigation phase and to broaden and detail the database of the Äspö site. The first part of the tunnel to 3 200 m was excavated using the drill-and-blast technique and the final 400 metres using the Tunnel Boring Machine (TBM) with a diameter of 5 metres. The underground excavations are connected to the Äspö Research Village, comprising offices, stores, laboratories, hoist and a ventilation building, by an access shaft and two ventilation shafts.

3.3.2 Geology and tectonics

During tunnel construction the rock-type distributions and fracture data were assessed in connection with the general geological mapping performed after each new tunnel section excavated. Core drillings provided supplementary information especially regarding fracture zone characteristics and the dispersion of grout in fractures was evaluated by means of TV-inspection using a Pearpoint flexiprobe system. Radar measurements and geophysical logging in boreholes were also performed for supplementary structural characterisation, and grouting of the tunnel was systematically documented. An overview of the geological documentation is available along 150 m tunnel sections.

Combining these data with those from the pre-investigation phase, discontinuities were divided into fracture zones (major: width >5 m; minor: width <5 m) and small-scale fracturing in the rock matrix between fracture zones. Three of the major sub-vertical fracture zones recognised from the pre-investigation phase, NE-1, EW-3 and EW-1, were further characterised and documented when intercepted by the excavations or by new boreholes from the tunnel (i.e. EW-1; *Fig.3-4*).

Drill core samples from the tunnel walls were analysed with respect to density and porosity of the rock matrix. Rock types were checked by means of microscopic modal analyses and fracture minerals were sampled and to some extent examined by means of x-ray diffraction (XRD) analyses (especially clay minerals).

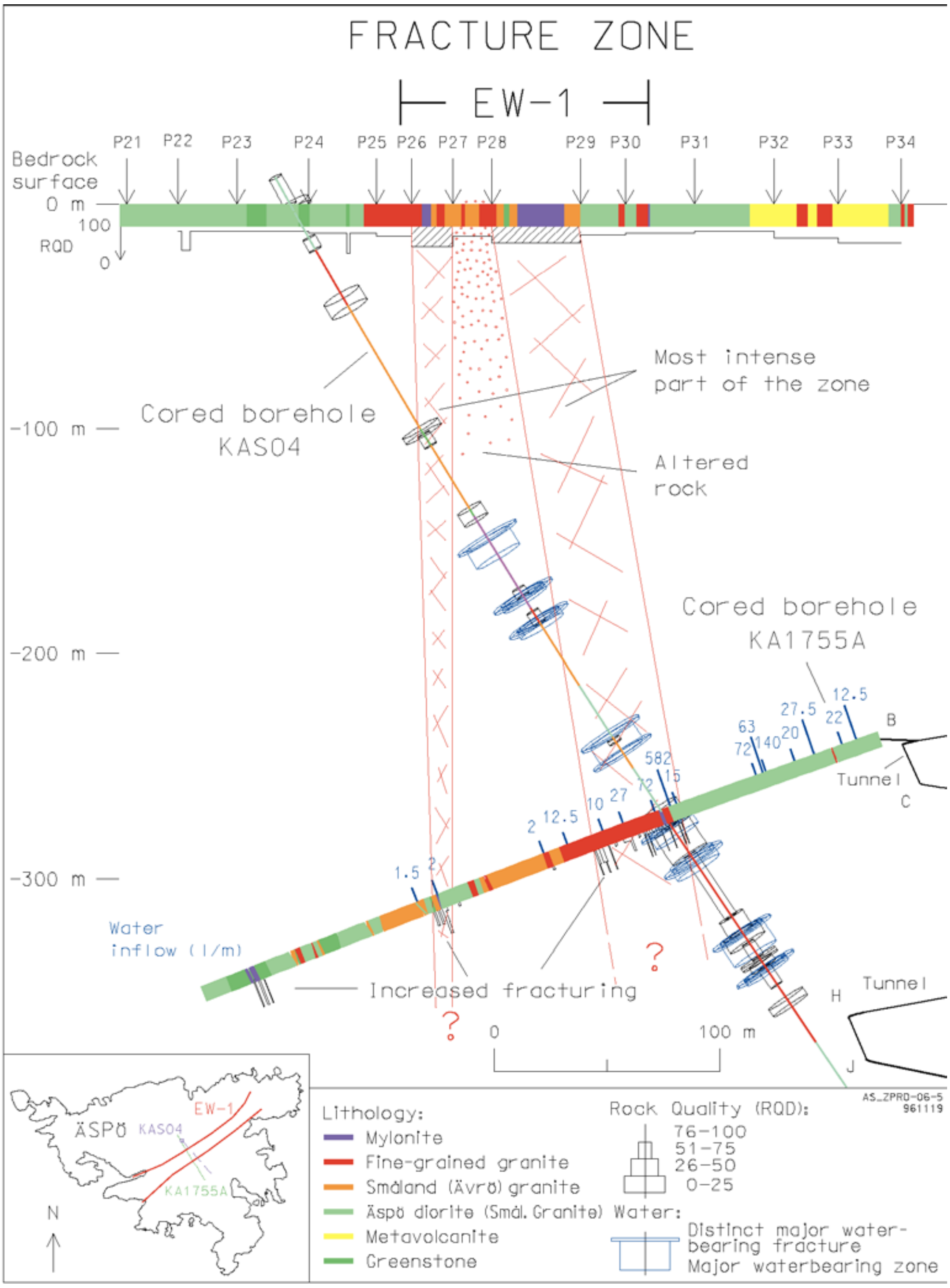


Figure 3-4. *Interpretation of fracture EW-1 based on surface and borehole observations from tunnel drilling (Stanfors et al., 1994).*

Following the construction phase the geological model was up-dated (to Model Stage 5) and this is illustrated partly below in Figure 3-5.

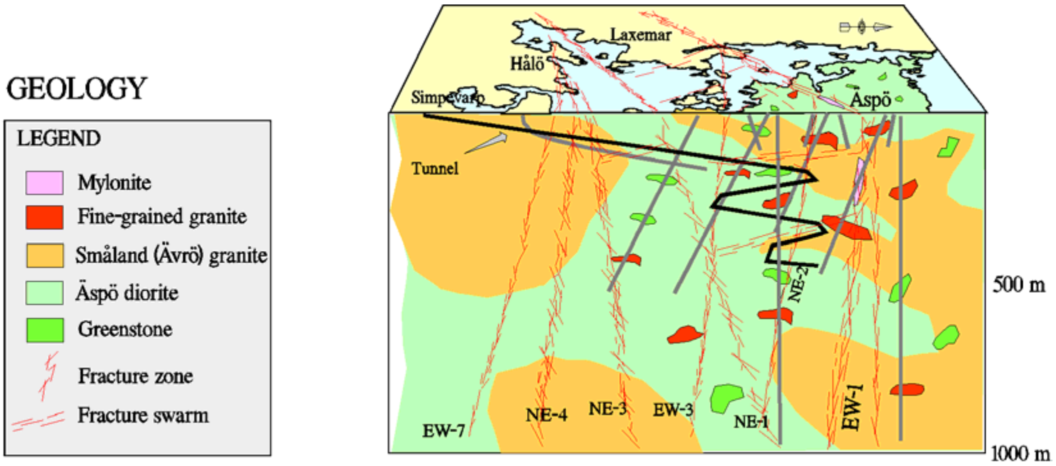


__Figure 3-5.__ Modified geological model following the construction phase (compare with Fig. 3-1) (Rhén et al., 1997a).

3.3.3 Hydrogeology

The construction phase contributed significantly in further characterising the different bedrock hydraulic domains. The geometry of these hydraulic conductor domains is mainly defined by the major fracture zones described previously although the minor fracture zones in the 'NNW-system' are also important conductors. A few hydraulic conductor domains were also added to the earlier model in order to explain some of the responses obtained in the hydraulic interference tests. A simplified model of the hydraulic conductor domains was made by fitting planes to the observations at the surface and in the boreholes. The evaluated transmissivities are generally in the range 10^{-6}-10^{-4} m^2/s with a median of about 10^{-5} m^2/s. The greatest transmissivities for these larger features correspond to the hydraulic conductor domains below the Baltic Sea and also for the minor fracture zone NNW-4. The largest transmissivity measured is approx. $4 \bullet 10^{-4}$ m^2/s for hydraulic conductor domain NE-1.

With respect to the hydraulic rock mass domains, tests from the southern part of Äspö, i.e. that bounded by the southern part of EW-1 and fracture zone EW-3, showed that at scales of 3, 30 and 100 m, there was no indication of decreasing hydraulic conductivity at the 0-500 m depth interval. Below 600 m depth the hydraulic conductivity decreases although this result is based only on one vertical borehole. If the data from the 1700 m deep cored borehole KLX02 on the mainland at Laxemar are included in the analysis, the hydraulic conductivity appears to decrease at a depth of 600 m below sea level.

The mapped water-bearing fractures and the grout-filled fractures (pre-grouted ahead of the tunnel face) in the tunnel are dominated by a subvertical fracture set striking WNW. This fracture set also has the highest frequency of all fracture sets. Hydraulic tests in probe holes drilled along the tunnel during excavation indicate that subvertical fractures striking approximately WNW and N-S are more transmissive than the others. Occasionally, single water conducting fractures in the hydraulic rockmass domains can be very transmissive and cause localised high flow rates into drilled boreholes.

These additional data resulted in a modified hydrogeological model (Stage 5) illustrated below (*Fig. 3-6*).

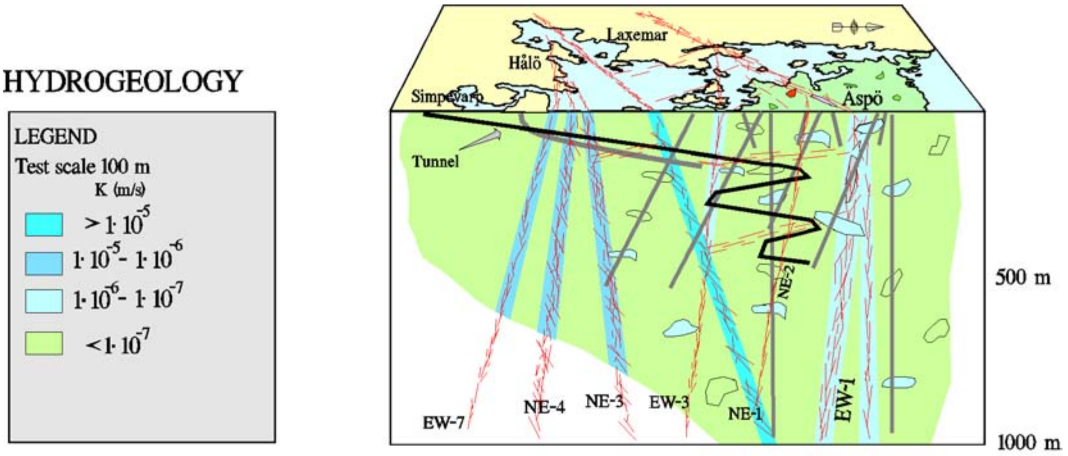


Figure 3-6. *Modified hydrogeological model following the construction phase (compare with Fig. 3-1) (Rhén et al., 1997a).*

3.3.4 Hydrogeochemistry

Excavation of the access tunnel and laboratory facilities has had a marked effect on the ‘undisturbed’ groundwater chemistry. Long-term monitoring of these effects has been carried out during and subsequent to construction from various levels in selected pre-investigation boreholes and at suitable control points along the tunnel section (Fig. 3-7); the majority of these control points coincide with hydraulically active fracture zones. Generally, excavation has resulted in a hydraulic drawdown causing younger, more surface-derived water to be circulated to greater depths; it has also led to an upconing of deeper, older, more saline water to shallower depths. More specific evaluation of the long-term monitoring along approximately the first 2900 m of the tunnel (Laaksoharju and Wallin (Eds.), 1997; Svensson et al., 2001) indicates that during construction:

- the groundwater along the 500-1000 m tunnel section changed from meteoric to a marine signature due to the fact that the tunnel starts under the landmass and continues under the sea towards Äspö island,
- the groundwater along the 1000-2000 m tunnel section showed an initial change from a marine to a meteoric/glacial/saline signature that later changed to a meteoric signature, reflecting that this tunnel section started under the sea, continued under Äspö island and then ended in the first spiral, and

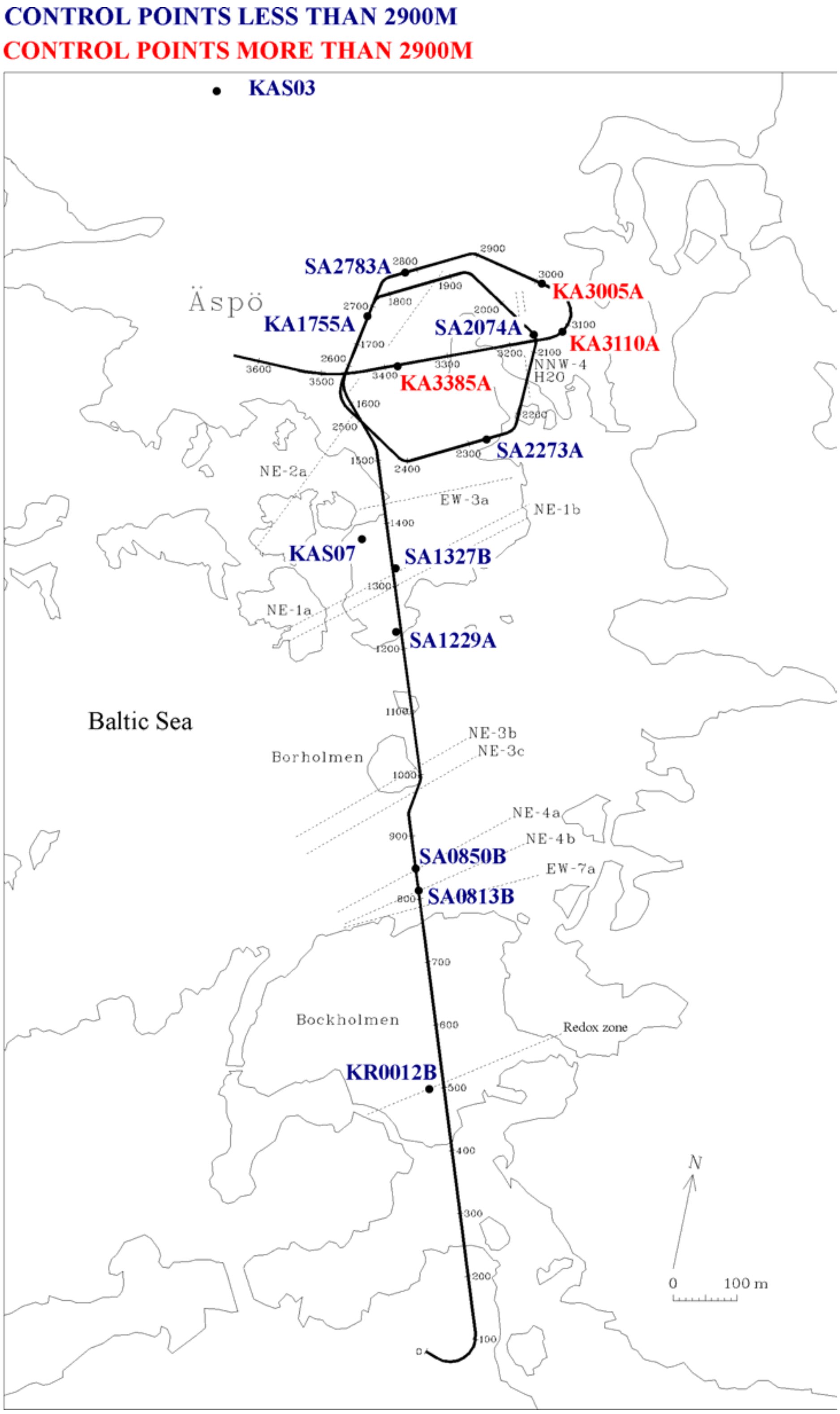


Figure 3-7. *Location and outline of the Äspö Hard Rock Laboratory in relation to the major fracture zones. Along the access tunnel and spiral ramp various control points (CP) are indicated; those in blue represent 0-2900 m, and those in red > 2900 m. Groundwater samples from these locations were used in the Task 5 modelling exercise. The control points >2900m were used for predictions (Svensson et al., 2001).*

- the groundwater along the 2000-2880 m section (which represents the distance from end of the first spiral to the beginning of the second spiral) changed from meteoric to marine and then increased in saline content from the mixing of groundwaters originating at greater depths.

In conclusion, the major observed changes in the groundwater chemistry simply reflect the intersection of the tunnel during construction with a series of hydraulic fractures and fracture zones of varying geometry and geographic location such that groundwater mixing from different sources has occurred. However, chemical reactions have also contributed, for example, the observed carbonate increase under the landmass areas is attributed to decomposition of organic matter and calcite dissolution, whilst under the sea the increase is due to sulphate reduction. Decomposition of organic matter and sulphate reduction has been biologically mediated.

To illustrate the changes in groundwater chemistry with time during tunnel construction, a series of time plots are presented in *Figure 3-8*. At several of the control points there is a clear variation in chemistry due to different mixtures of the four main groundwater end members: Meteoric Water, Baltic Sea Water, Glacial Water and Äspö Brine. For example in fracture zone NE-2.1 a marked decrease in Glacial Water is compensated by an incursion of both modern Baltic Sea and Meteoric waters. Some of the other control points also reflect this trend to a lesser degree whilst others show little variation with time (e.g. NE-3).

These additional data resulted in a modified hydrogeochemical model (Stage 5) illustrated below (*Fig. 3-9*).

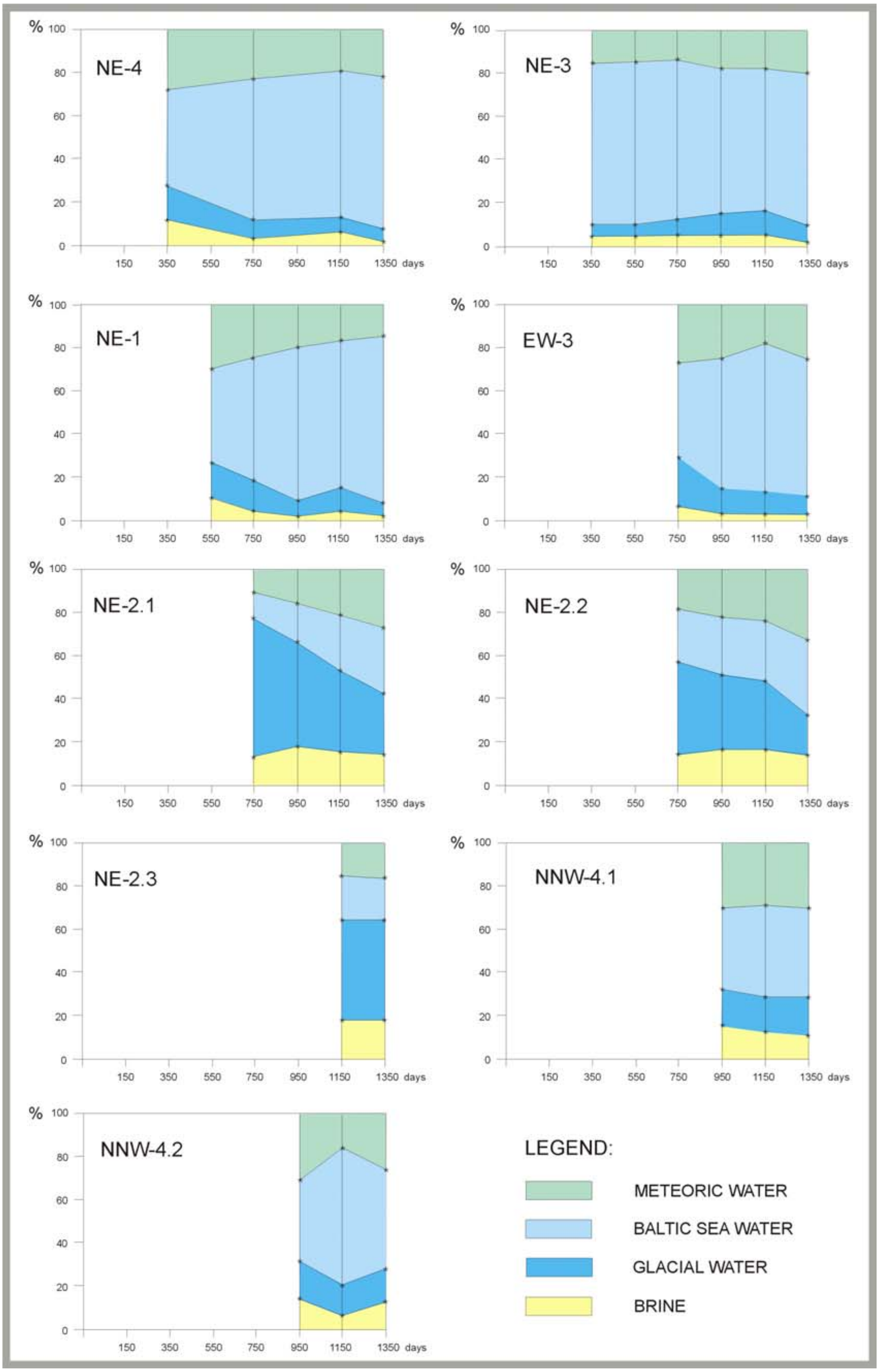


Figure 3-8. *Calculated mixing proportions of groundwater end members based on time-series measurements at selected control points along the Äspö tunnel (Rhén et al., 1997b).*

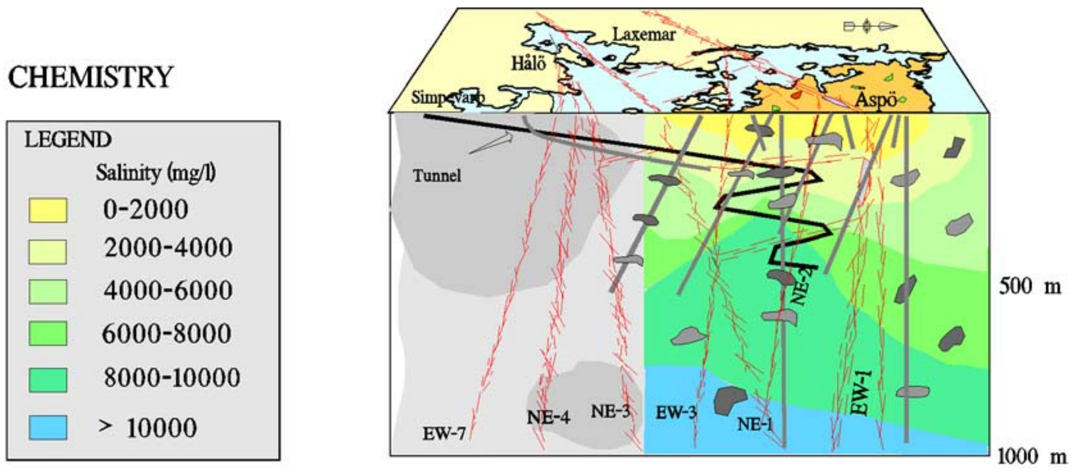


Figure 3-9. *Modified hydrogeochemical model following the construction phase (compare with Fig. 3-1) (Rhén et al., 1997a).*

3.4 Groundwater-flow modelling

As described above, conceptual modelling has been carried out prior to, and at various stages during the tunnel excavations. With respect to the 'undisturbed' conditions, i.e. based solely on data obtained from the pre-investigation boreholes, *Rhén and Wikberg (2000)* summarised the status reached in 1996. By integrating geology, hydrogeology and hydrochemistry it was possible to qualitatively indicate the major groundwater flow directions and the chemical changes in groundwater composition. During tunnel excavation the hydrochemistry, when compared with the 'undisturbed' pre-investigation conditions, shows a drawdown of low salinity, more surface-derived groundwaters and an upconing of higher salinity groundwaters.

'Undisturbed' and disturbed flow field conditions below Äspö have also been modelled using a stochastic continuum approach (PHOENICS code) at a *regional (Svensson, 1997a)* and site *(Svensson, 1997b)* scale. The site scale groundwater flow model was used to illustrate the changes in recharge and discharge patterns due to the excavations, and also to show the changes in the salinity distribution. A N-S section through the salinity distribution model, oriented to cut the centre of the tunnel spiral, is presented in Figure 3-10. The figure shows that the maximum depth of the fresh water lens (0.1% salinity isoline) is about 300 m below Äspö under natural conditions. Under disturbed conditions the groundwater flow into the tunnel changes the distribution of the salinity mainly below Äspö island, where upconing of saline water is clearly observed.

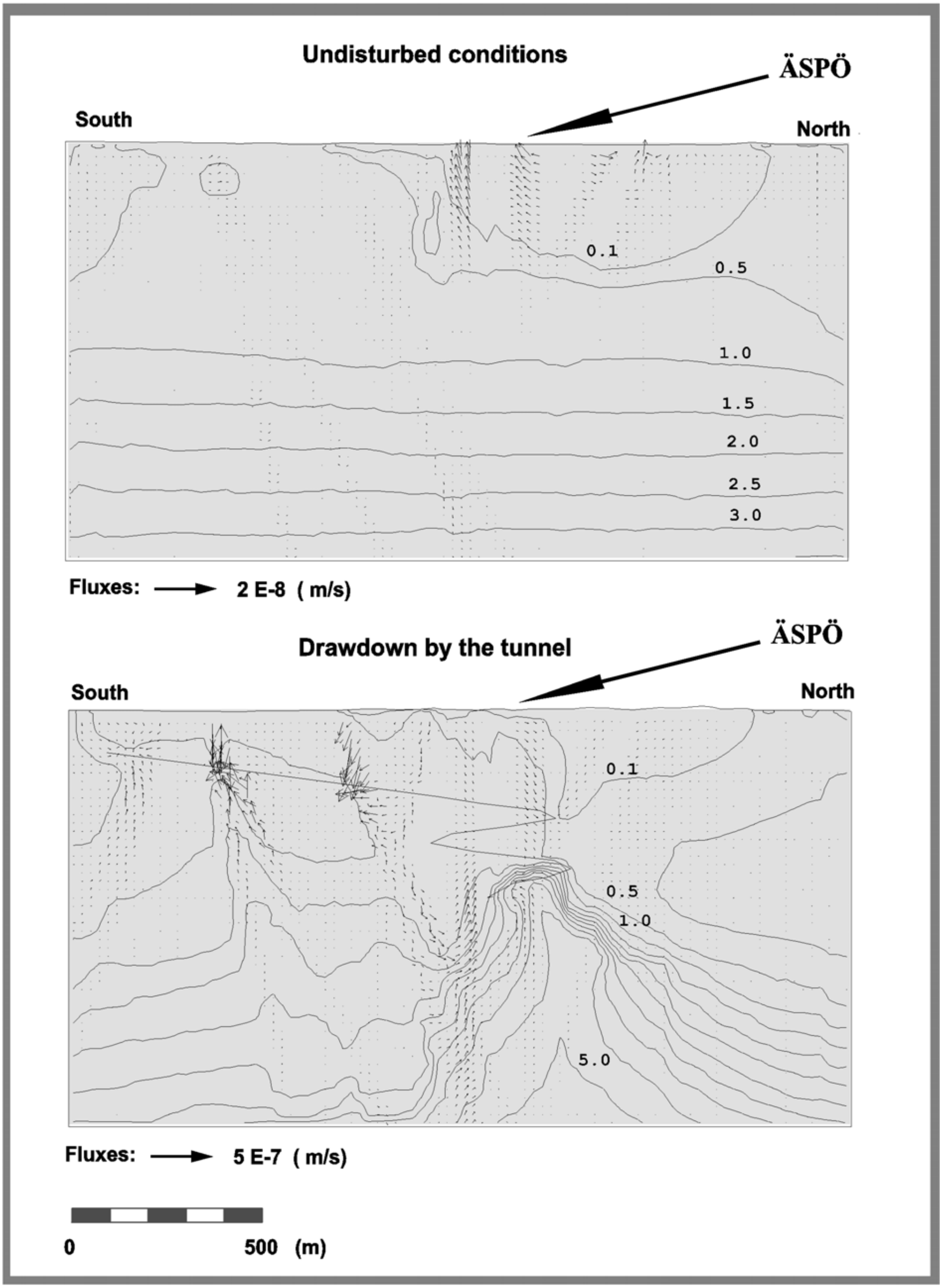


Figure 3-10. *Site scale groundwater flow model under Äspö showing salinity fields in % and groundwater flow directions. The N-S vertical section shows natural conditions in the top figure and disturbed conditions below. The flow field from the surface to 20 m depth is not shown (Rhén et al., 1997a).*

3.5 M3-derived hydrochemical data

3.5.1 General

The principles of M3-derived hydrochemical data are outlined at this juncture since M3 data are used as input to all the Task 5 modelling exercises and is referred to repeatedly throughout the report.

M3 stands for Multivariate Mixing and Mass balance and is a statistical method 'to analyse variations in groundwater compositions so that the mixing components, their proportions, and the effects from chemical reactions are revealed' *(Laaksoharju et al., 1999).* It has been developed as part of SKB's future strategy to hydrogeochemical site characterisation investigations and is intended to complement more commonly used evaluation methods such as standard trilinear plots and geochemical equilibrium/kinetic reaction modelling. The Äspö HRL site has proved a suitable location to develop M3 because hydrodynamic effects initiated during and since the last glaciation(s) have resulted in widespread mixing of groundwaters of different origins, especially down to a depth of 500 m, i.e. to the present level of the underground laboratory facilities. Furthermore, since an integral part of site characterisation studies is to simulate/predict groundwater conditions resulting from the construction of a potential repository, dynamic mixing processes are expected to dominate during this construction phase thus underlining further the potential use of M3 modelling.

3.5.2 M3 model

The M3 method, being mathematically based, has the advantage of objectivity when classifying large sets of hydrochemical data, although the initial and final choice of groundwater end members requires close familiarity with the system being investigated. Further features of M3 include the fact that model construction is based on all the measured data and therefore all the samples are compared by using the same model, and that both conservative and non-conservative species are used. It should be noted, however, that the M3 model is only concerned with water comparison data and no space or time restraints, or geological and hydrogeological information, are included in the model.

Based on *Svensson et al. (2002),* the modelled approach used at Äspö consisted of three steps (*Fig. 3-11*):

1. Principal Component Analysis (PCA) was used to cluster and summarise the information and finally construct an ideal mixing model for the site under investigation. Generally the major constituents were used (Cl, Ca, Na, Mg, K, SO_4 and HCO_3) together with the environmental isotopes (^3H, δ^2H and $\delta^{18}O$). Only the first two principal components were used since they describe around 70% of the information; the third or fourth principal components were considered to contain information less useful to mixing and reactions. By visualising the data as a PCA plot it was possible to make a first attempt to identify the main reference (or end member) groundwater compositions from the cluster distributions. Lines were drawn between the reference waters to construct a polygon, thus the observations defined by the

polygon could be described in terms of mixing and reactions by the selected reference groundwaters.

2. Mixing calculations were used to determine the mixing proportions. These describe the contribution of each reference groundwater to each of the sampled waters that plot within the polygon. They can also be used to indicate the origin, major flow paths and flow directions and possible residence times of the groundwaters. The average range of uncertainty at Äspö for the M3 calculations was ± 10% at a 90% confidence level when calculated over the polygon of interest; greater uncertainties can therefore influence 10% of the samples.

3. The mixing proportions calculated in Step 2 were used to recalculate concentrations for the selected chemical species that would occur if they were determined only by mixing. Mass balance calculations were then used to define the sources and sinks for the different chemical species that deviate from the ideal mixing model used in the mixing calculations. A positive deviation indicates a source (or addition) to the groundwater system, a negative deviation a sink (or removal) from the groundwater system. The accuracy of the calculations was ±10% from the reported values.

The positive or negative deviation from the ideal mixing model indicated from the mass balance calculations in Step 3 suggested the influence of reactions on the groundwater system (*Fig. 3-11*). Six major geochemical reactions are known to be active in the Äspö groundwater system, each resulting in gains and losses of chemical species. By relating these changes to the respective ionic deviations from the ideal mixing model, a qualitative indication of the relevant chemical reactions could be determined. The six major Äspö reactions identified from earlier studies at the site included:

- Organic decomposition: Mostly associated with meteoric groundwater and restricted to the unsaturated zone; oxygen is consumed and results in a gain of HCO_3.

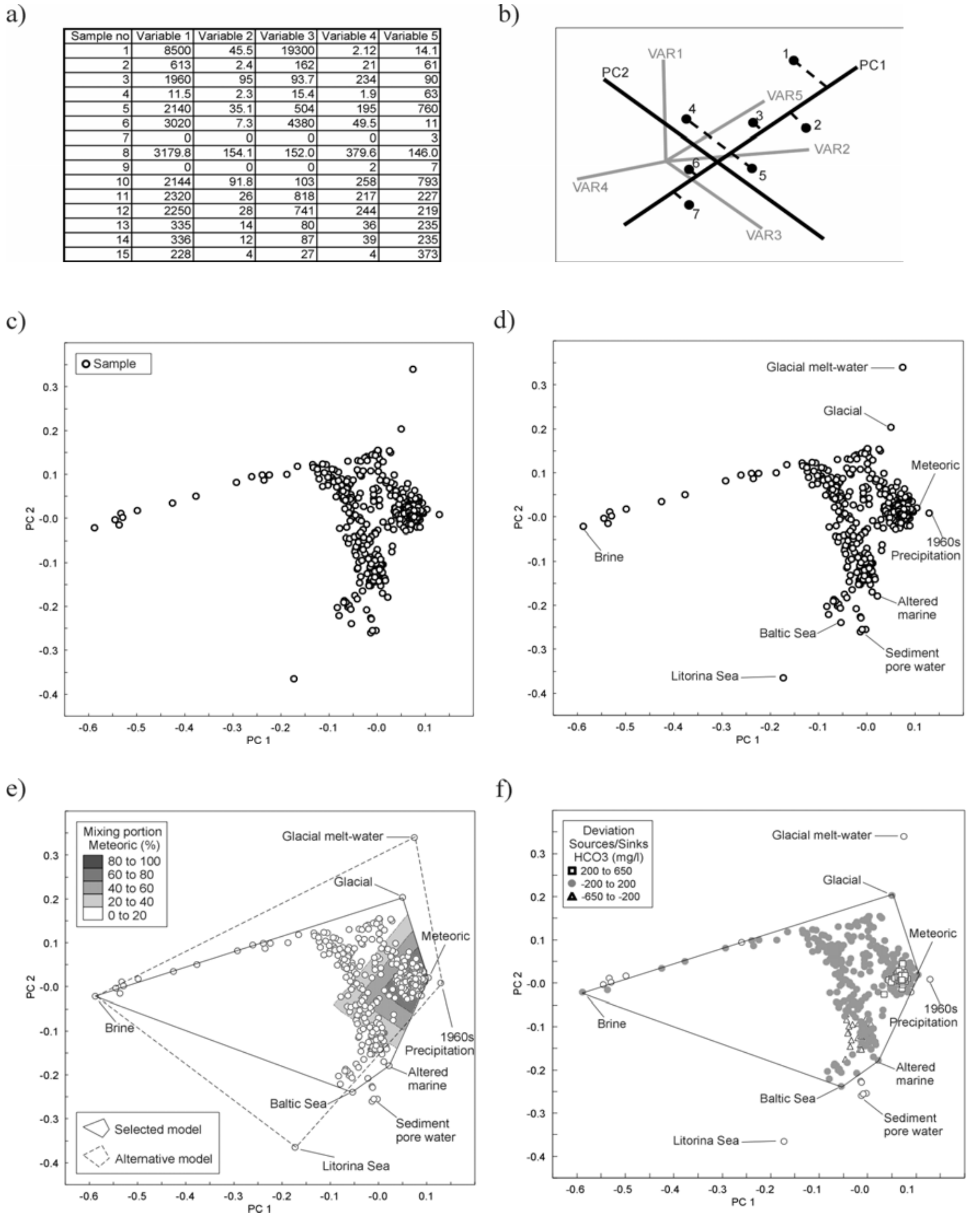
- Organic redox reactions: Mostly associated with recharging meteoric groundwater in the upper part of the bedrock; oxidation of organic matter causes a reduction of Iron (III) resulting in a gain of HCO_3 and Fe.

- Inorganic redox reactions: Mostly associated with recharging meteoric groundwater in the overburden and upper part of the bedrock; oxidation of sulphide (i.e. pyrite in the soil and fracture minerals) resulting in a gain of SO_4.

- Dissolution and precipitation of calcite: Occurs in the upper (dissolution) and lower (precipitation) parts of the bedrock and may be associated with all groundwater types; dissolution results in a gain of Ca and HCO_3 and precipitation in a loss of Ca and HCO_3 in the surrounding groundwaters

- Ion exchange: Occurs throughout the bedrock mass and may be associated with all groundwater types; cation exchange with solid substrate (e.g. clays) resulting in a change of Na/Ca ratios.

- Sulphate reduction: Occurs in the upper bedrock associated with marine-derived groundwaters; microbe activity in the presence of organics reduces sulphate to sulphide resulting in a decrease in SO_4 and an increase in HCO_3.



Sample no	Variable 1	Variable 2	Variable 3	Variable 4	Variable 5
1	8500	45.5	19300	2.12	14.1
2	613	2.4	162	21	61
3	1960	95	93.7	234	90
4	11.5	2.3	15.4	1.9	63
5	2140	35.1	504	195	760
6	3020	7.3	4380	49.5	11
7	0	0	0	0	3
8	3179.8	154.1	152.0	379.6	146.0
9	0	0	0	2	7
10	2144	91.8	103	258	793
11	2320	26	818	217	227
12	2250	28	741	244	219
13	335	14	80	36	235
14	336	12	87	39	235
15	228	4	27	4	373

__Figure 3-11.__ A schematic visualisation of the different steps in the M3 modelling: a) Data table containing groundwater compositions. b) The principle for principal component analysis; seven groundwater samples and their location in the multivariate space (VAR1-VAR5) and their projection on the principal component 1 (PC1) are shown. c) The result of the principal component analysis showing principal components 1 and 2. d) Selection of possible reference waters; the other groundwaters are compared to these. e) Mixing calculations; the linear distance of a sample to the reference waters (e.g. the proportions of Meteoric water (%)) are calculated in the figure for the selected ideal mixing model; the alternative model uses a new set of reference waters. f) Mass balance calculations; the sources and sinks (mgL) of carbonate (HCO_3) are shown which cannot be accounted for by using the ideal mixing model (Svensson et al., 2002).

The M3 model, in common with all geochemical evaluation models, is no better than the quality of the input data and conceptual ideas. *Svensson et al. (2002)* list several causes for uncertainty in the Äspö data which covered:

- *Sampling*; possible disturbance of samples due to borehole activities (estimated uncertainty of ±10% from the real, undisturbed value);
- *Analysis;* lack of precision/accuracy (range of 1-5% deviation in values between laboratories);
- *Conceptualisation*; selection of erroneous number and type of end members (M3 model detection limit is a mixing portion <10%), and mixing of samples that are not mixed (uncertainty range in the mixing portion calculations is ±0.1 mixing unit);
- *Methodology*; model oversimplification and bias; these may influence the accuracy of the mixing portion calculations (uncertainty of ±0.1 mixing unit).

The M3 modelling approach has been widely applied to the Äspö site at all stages of investigation and tested also at other sites characterised by contrasting climate, geology and groundwater conditions (see *Laaksoharju, 1999* and references cited therein). The importance of M3 to Task 5 lay in its direct input, in the form of calculated mixing ratios at each of the control points, to the hydrodynamic modelling exercises thus providing some common ground for model comparison.

3.6 Databases

There is an immense amount of data available from the Äspö site covering the pre-investigation and construction phases of the Hard Rock Laboratory. These data have been systematically archived in the SKB SICADA Database. The hydrogeochemical data for the pre-investigation phase have undergone a thorough and selective evaluation of their suitability (i.e. degree of representativeness) for modelling input *(Smellie and Laaksoharju, 1992).* For the construction phase the majority of the hydrogeochemical data have been included since any deviation from the undisturbed pre-investigation conditions is of potential importance in interpreting the degrees of mixing/reaction etc. during the construction phase.

Complete details of the data sets provided for the Task 5 modelling exercise are given in Appendix 1.

4 Modelling: Background perspective and Task 5 issues

4.1 General approaches

Most models require a common set of physical and/or chemical parameters as input. The difference between one approach to another is the number of parameters that can be handled and how the model mathematically integrates and adjusts these parameters to produce a realistic representation of the area in question. As a general background to the Task 5 modelling exercise, a brief outline is presented below of the various hydrodynamic and hydrogeochemical modelling approaches used in Task 5, the input data normally required, and the type of modelled information produced.

4.1.1 Hydrodynamic modelling

Groundwater flow modelling of heterogeneous soil and highly heterogeneous rock can be based on several concepts. Stochastic continuum for both soil and rock is common. The rock can be modelled with stochastic distributed 2D-feature (Discrete Fracture Network, DFN) or a hybrid; stochastic distributed 2D-features as a base for generating properties in a continuum code. The parameterisation of the groundwater flow models based on these concepts is slightly different but in principal it is the same equations that are used for calculation of the advective flow. The basic equations for advective flow including density driven flow are as follows:

Equation of motion:

$$q = -\frac{k}{\mu} \cdot \left(grad(p) + \rho \cdot g \cdot grad(z) \right) \tag{4-1}$$

The continuity equation (mass conservation) is given by:

$$div(\rho \cdot q) + \frac{d(\rho \cdot n)}{dt} + \rho \cdot Q = 0 \tag{4-2}$$

Transport equation:

$$div(D\rho \cdot grad(C) - C\rho \cdot q) = \frac{\partial(\rho n_e C)}{\partial t} + Q_s \rho \cdot C_s \tag{4-3}$$

The equations of state are:

$$\rho = f(T, C, p) \tag{4-4}$$

$$\mu = f(T, C, p) \tag{4-5}$$

Mean velocity of the advective flow (average linear velocity):

$$\mathrm{v}_a = \frac{\mathrm{q}}{n_e} \tag{4-6}$$

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

As seen in the equations a few transport parameters (Dispersion coefficient (Hydrodynamic dispersion and diffusion), kinematic flow porosity) for conservative transport of salt is needed. Chemical species can be transported by the groundwater flow and the evolution of the chemical composition along a flow path may be controlled by a number of different processes. Some possible processes and the application in the transport equation 4-3 can be found in the literature.

These equations above form the basis for calculating water flow taking into account pressure, temperature and density conditions. The permeability is given by the properties of the pore system and the dynamic viscosity determines the properties of the fluid. If the density effect is neglected the above equation can be simplified as below.

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

Equation of motion:

$$q = -\frac{k \cdot \rho \cdot g}{\mu} \cdot grad\left(\frac{p}{\rho \cdot g} + z\right) = -K \cdot grad\left(\frac{p}{\rho \cdot g} + z\right) = -K \cdot grad(h) = K \cdot i \tag{4-7}$$

The continuity equation:

$$-div(q) \approx \frac{S_S}{\rho \cdot g}\frac{d(p)}{dt} + Q \approx S_S \frac{d(h)}{dt} + Q \tag{4-8}$$

and $\mathrm{K} = \dfrac{\rho \cdot \mathrm{g} \cdot \mathrm{k}}{\mu}$ (4-9)

and $\mathrm{S_s} = \rho \cdot \mathrm{g}\,(\alpha_\mathrm{b} + \mathrm{n} \cdot \beta_\mathrm{l})$ (4-10)

(Hydraulic conductivity (K), Specific storage coefficient (S_s). S_s depends on the compressibility of the porous medium (α_b) and the compressibility of the liquid (β_l))

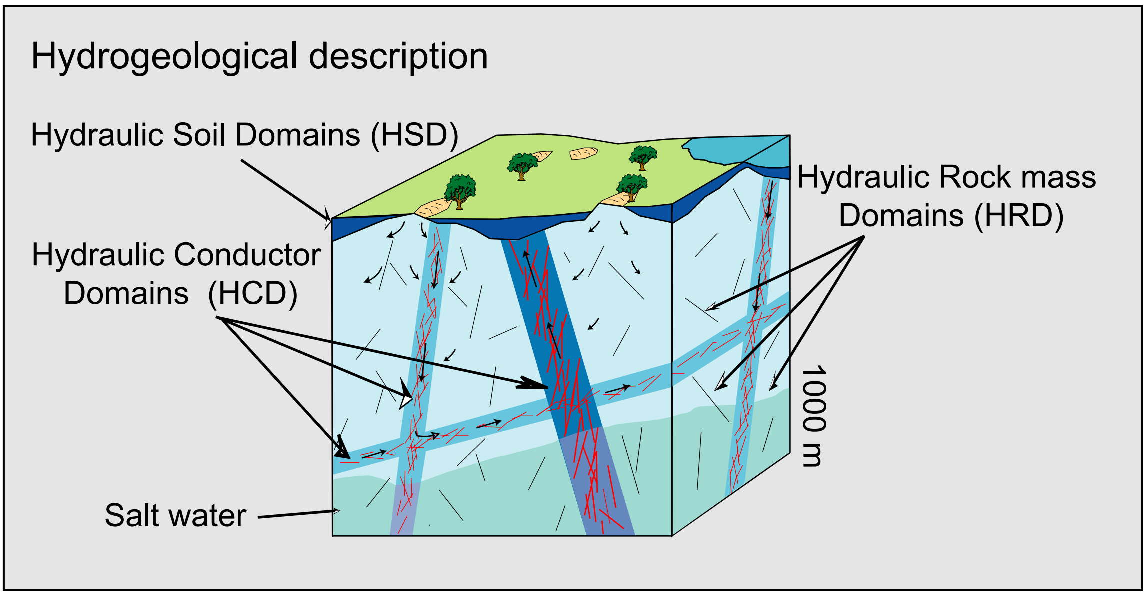


***Figure 4-1.** Schematic visualisation of main geometrical units (HSDs, HRDs, HCDs) in the hydrogeological description (SKB 2001).*

In a DFN model 2D features are spatially interconnected. Each individual feature may be assumed to have constant properties or have a stochastic distribution. The primary parameters assuming constant fluid properties are transmissivity (T) and Storage coefficient (S).

Driving forces for the groundwater are the levels of the water table and the lakes and sea. The levels of these are coupled to precipitation/evapotranspiration as well as the properties of the geosphere.

The processes considered important are incorporated into a geometric framework. During the site investigations for the Äspö HRL it was decided that the larger fracture zones had a significant impact in calculating the groundwater flow and construction of the laboratory, and should as far as possible be defined deterministically in space. As hydraulic elements they were named Hydraulic Conductor Domains (HCD). The rock mass separating the fractures was called the Hydraulic Rock mass Domains (HRD and the overburden referred to as the Hydraulic Soil Domain (*Fig. 4-1*).

The internal structure of these domains may be modelled in several ways; as Continuum (C) (alternatively Stochastic Continuum (SC)), Channel Network (CN) (which is more similar to ‘C’ concerning flow but may differ concerning transport) and Discrete Fracture Network (DFN) (see *Figure 4-2*).

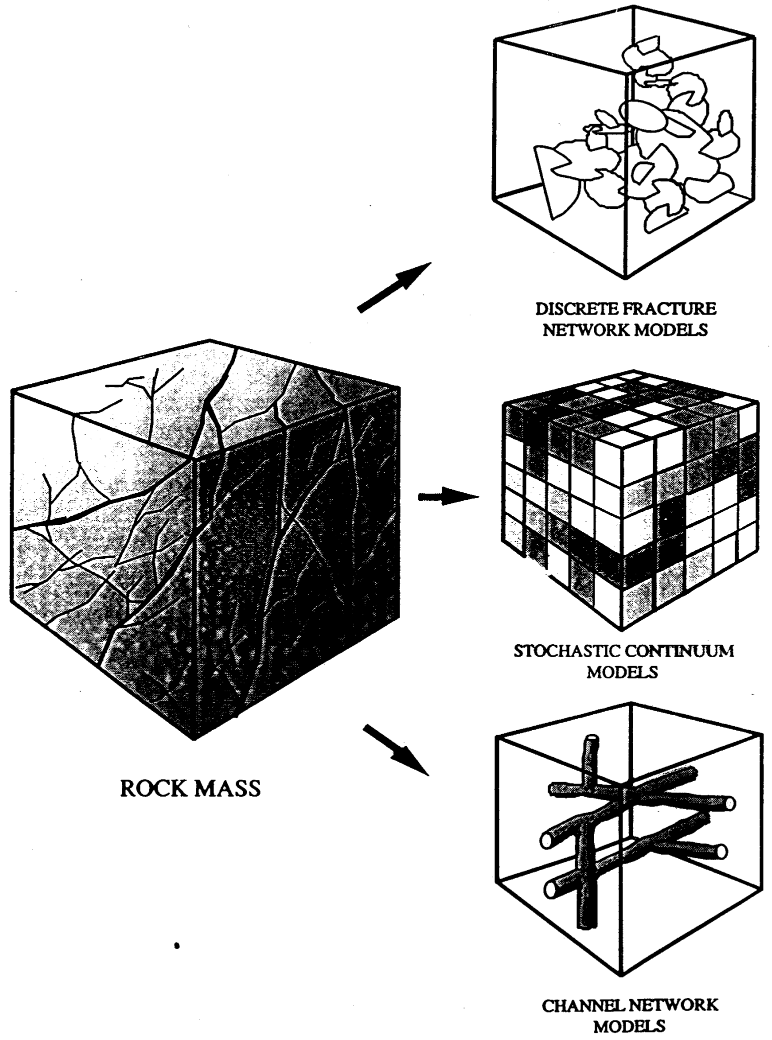


***Figure 4-2.** Schematic visualisation of main approaches for modelling of internal geometrical hydraulic domains (Geier et al., 1992).*

The flow properties of the pore structure in crystalline rock are determined by the fracture structures. The flow properties depend both on the flow properties of each fracture and how these fractures are interconnected, but above all are dependent on the fracture aperture and on its internal surface structure. Consequently, it is likely that most of the flow is channelled along the fracture planes and transport outside the flow channels is due to diffusion, thus the “kinematic porosity” is less than the “total fracture porosity”. *Svensson (2001)* has also shown that the flow rates within the fracture plane can differ greatly and, if water of different densities is flushed through the fracture system, water bodies can be obtained within the fractures that have quite different densities. Both of these factors can have a significant effect on the observed chemical composition of the flowing groundwater. Dispersion of a solute in a fractured system is probably an effect of several processes occurring on different geometrical and time scales. The observed “Dispersion Coefficients” should therefore be handled with care and be integrated with how the properties are assigned to the hydraulic domains. Sorption/desorption on the fracture surface and rock matrix are sometimes relevant for the transport.

The rock matrix hosting the fractures normally contain microfracures with very small apertures. Flow through the matrix is generally considered negligible but transport by diffusion is sometimes considered to be a relevant process.

The processes included in the modelling by each group are briefly described in section 4.3.

4.1.2 Hydrogeochemical modelling

Hydrogeochemical modelling of a typical Fennoscandian groundwater system schematically shown in *Figure 4-3* can be divided into five main categories: a) simple mixing models, b) mass balance models, c) geochemical equilibrium models, d) geochemical kinetic models, and e) geochemical reaction transport models. Simple mixing models are based on the measured concentrations of two (or more) groundwater compositions which are mixed together to derive the final composition. The mixing proportions are normally derived from a mobile (i.e. chemically conservative) element of the groundwaters mixed, such as chloride. Hydrogeochemical mixing modelling using the M3 method has already been addressed in sub-section 3.4 and will not be further mentioned here; alternative approaches to M3 are described below in section 5.7.

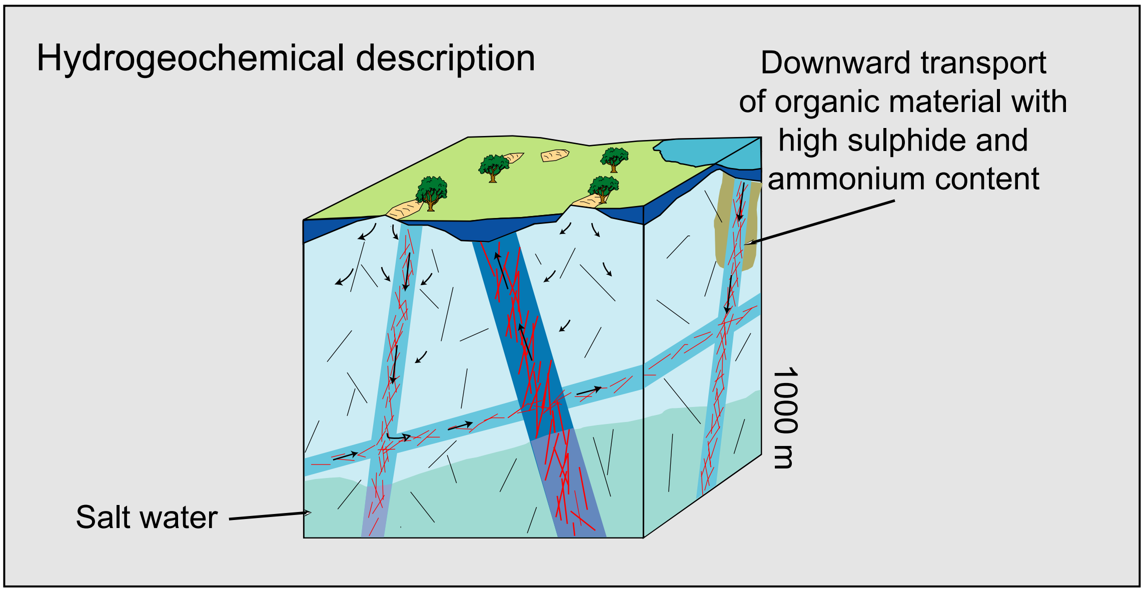


Figure 4-3. *Schematic visualisation of major groundwater types used in the hydrogeochemical description. Groundwater compositions will result from mixing and reaction processes along different recharge pathways through a crystalline rock environment (SKB, 2001)*

Mass balance models are used to identify and quantify mineral reactions that might occur between two groundwaters sampled along a flow path. Ideally, such models are used in combination with information obtained from geochemical equilibrium modelling. An integral part of chemical equilibrium, kinetic and reaction transport models is the speciation of the aqueous phase, i.e. the distribution of aqueous species among free ions, ion pairs and complexes, and the mass transfer between two or more phases, such as the precipitation or dissolution of minerals. Depending on the system under investigation the modelling can be performed assuming that chemical equilibrium is attained among the aqueous species as well as between the aqueous and solid phases (equilibrium models) or that speciation and mass transfer are controlled by reaction kinetics (kinetic modelling). Geochemical equilibrium models have been most developed and widely used in hydrogeochemical studies of deep aquifer systems where the mean residence time of groundwater is long compared to the reaction kinetics. Geochemical kinetic models are mostly used in surface and near-surface water environments and groundwater systems where the mean residence time of the groundwater is short compared to the reaction kinetics.

Generally most available independent hydrogeological and hydrogeochemical codes are not fully coupled. However, reaction transport models which couple speciation and mass transfer with fluid flow are increasingly being developed to understand and predict the spread of pollutants, not least as an integral part of the long-term performance assessment of deep, geological repositories for radioactive waste disposal (e.g. CORE^{2D} model used by ENRESA; see section 5.5.5).

Mass balance modelling

Mass balance calculations were first used by *Garrels and MacKenzie (1967)* to construct "reverse weathering" reactions to describe the weathering of a granitic rock from observed groundwater data. This type of modelling was further elaborated by *Plummer and Back (1980)* who used the approach to calculate the masses of plausible minerals and gases that enter or leave the aqueous phase to account for the observed changes in two groundwater compositions along an evolutionary path. The mass balance or inverse geochemical modelling approach was successfully developed and applied, for example to the Floridan and Madison limestone aquifers *(Plummer and Back, 1980; Plummer et al., 1990)* by applying the computer code BALANCE *(Parkhurst et al., 1982).* The modelling concluded that in these systems calcite is first dissolved and then precipitated further along the flow-path, while dolomite and gypsum dissolve irreversibly.

The mass balance modelling approach was further developed with the code NETPATH *(Plummer et al., 1991, 1994).* This code allows computation of mixing proportions of up to five initial waters and net geochemical reactions that can account for the observed composition of the final water. In addition, isotopic data might be included as additional constraints. Every possible geochemical mass balance reaction model is examined between selected evolutionary waters for a set of chemical and isotopic constraints, and for a set of plausible chemical sinks and sources (e.g. mineral phases and gases) in the system. The calculations are of use in interpreting geochemical reactions, mixing proportions, evaporation and (or) dilution of waters, and mineral mass transfer in the chemical and isotopic evolution of natural and environment waters *(Plummer et al., 1991, 1994).* The computed precipitation from the dissolution of a mineral phase must be consistent with the saturation state of this mineral in the final water in order to become a valid model.

Geochemical equilibrium modelling

Traditionally, mathematical models developed to evaluate and understand natural aqueous geochemical systems have been based on the application of equilibrium thermodynamics. The initial stages of geochemical modelling go back to the classic paper by *Garrels and Thompson (1962)* on the speciation of seawater where they presented a thermodynamic model for the distribution of aqueous species in seawater. This model allowed, for the first time, a prediction of mineral saturation states (and mineral solubility) in a complex mixed-electrolyte solution by the simultaneous solving of sets of equations relating the activities of dissolved components to equilibrium with dissolved complexes and solid phases. This approach was further applied to the type of large-scale, heterogeneous sedimentary aquifer systems being studied at that time where the reaction kinetics of the major minerals involved are fast compared to the mean residence time of the groundwater and where there is a considerable time span available for completion of the various reactions. The assumption made, in other words, was that any reaction that reasonably could be expected to reach equilibrium in the aquifer system would do so. Simple examples of this type of model were applied successfully to carbonate systems (e.g. *Garrels and Christ, 1964).* Such aqueous speciation models are based either on the approach of an ion association model (for solutions with ionic strengths up to about that of seawater) or on specific interaction models (for solutions with ionic strengths above that of seawater).

A major difficulty with the early equilibrium thermodynamic models was the evaluation of systematic changes in groundwater composition along its flow-path, observed from many of the aquifer systems. The theoretical framework for the prediction of water-rock interaction along a flow-path and the adaptation of the calculation procedure to the computer was pioneered by Helgeson and co-workers *(Helgeson 1968; Helgeson et al., 1969, 1970).* Since then considerable progress has been made in the quantitative description of water-rock interactions *(e.g. PHREEQE: Parkhurst et al., 1980; EQ3/6: Wolery, 1979; Wolery et al., 1990)* also introducing the possibility of addressing ion exchange reactions, surface chemical factors and the influence of many organic complexes *(e.g. PHREEQC: Parkhurst and Appelo, 1999; EQ3/6: Wolery et al., 1990).*

Chemical reaction kinetic modelling

The basis of chemical reaction equilibrium modelling is that thermodynamic chemical equilibrium prevails in the system being modelled. However in many surface to near-surface groundwater conditions (e.g. active recharge weathering processes; active microbial activity), or, where deeper groundwater systems are disturbed (e.g. due to underground excavations) or the groundwater residence time is short compared to the mineral dissolution kinetics, equilibrium may not be achieved (or may be disturbed) and some reactions will be mainly controlled by kinetic considerations. Consequently, it is necessary to test the system under study. Some hydrogeochemical evaluation strategies use thermodynamic reaction path calculations to test the thermodynamic feasibility of reaction models derived from the mass balance calculations *(e.g. Pitkänen et al., 2001).* Reaction path calculations can better identify where equilibrium is not accomplished and kinetic information is required. Recently, reaction kinetics were included into already existing codes *(e.g. PHREEQC: Parkhurst and Appelo, 1999)* or geochemical reaction transport codes *(such as e.g. MPATH: Lichtner, 1985, 1988; OS3D: Steefel and Yabusaki, 1996).*

Geochemical reaction transport modelling

Several one-dimensional codes which couple, directly or indirectly, the transport of solutes in groundwater with solid phase reactions have recently been developed as process models to interpret or to scope future chemical changes associated with, for example, the short-term evolution of pollution plumes and the long-term performance of radioactive waste repository systems. These models impose further constraints on the transport of reactive solutes and on the development of system parameters (e.g. pH, major cations, redox). The models directly or iteratively couple equations formulating flow and mass transport, chemical equilibrium for major species and sorption. Chemical reaction kinetics, including 'kinetic sorption', has also been incorporated by some models. The role of chemical equilibrium for some trace solutes, including radionuclides, is not yet well understood whereas others such as uranium have been studied extensively in different geochemical environments.

The available codes address various aspects of the following chemical processes:

- thermodynamic equilibrium controlling major hydrochemical parameters and reactive mineral phases;
- kinetic reaction controls on hydrochemistry and solute transport;
- sorption, reversible or with kinetic controls, influencing transport of major and trace solute species;
- irreversible sorption, mineral precipitation or co-precipitation, of trace solutes.

Examples of some computer codes which couple reaction and flow include CHEQMATE; CHEMTARD, CHEMFRONTS, PRECIP, STELE, HYTEC, MPATH, OS3D.

Model limitations

Hydrogeochemical models in general, and hydrogeochemical mass balance (and kinetic reaction) models in particular, are no better than the quality of the input data. For example, a failure to analyse for all dissolved species and/or not allowing for analytical error, means that groundwater analyses are rarely exactly charged balanced. In addition, the validity of geochemical models depends on a certain amount of 'expert judgement' to select the appropriate mineral phases to be included in the model, in particular only those phases present in the system should be modelled. Furthermore, the actual composition of these phases should be known. As pointed out by *Plummer et al. (1991)*, 'Geochemical modeling should not be separated from an aggressive effort to study the mineralogy and petrology of the system'.

Reliability of the thermodynamic databases, used for both equilibrium and kinetic calculations, are of paramount importance. Consequently, in parallel with model development there have been continuous additions, modifications and improvements to the databases which have significantly increased the confidence of the modelled calculations. Several databases are in existence and modellers tend to have their own preferences.

Plummer et al. (1983) and Plummer (1984) also emphasise that geochemical modelling rarely leads to unique solutions; its strength is in eliminating reaction models from further consideration.

Finally, it is important to note that the effects of hydrodynamic dispersion are not explicitly accounted for in all of the reactive transport models. Compositional mixing effects due to dispersion cannot be separated from the analytical data. Although this effect is not considered important in large-scale sedimentary aquifer systems, it may have consequences in a fractured crystalline bedrock were groundwater movement may be more dynamic and the geometry and geographic location of the fracture systems may result in mixing and dispersing waters from different origins *(e.g. Steefel and Lichtner, 1998).* Furthermore, groundwater sampling procedures in a fracture flow environment may also initiate mixing, in addition to representing a rock volume of varying dimensions (reflecting variations of hydraulic conductivity) rather than a specific point. How representative are such groundwater samples when used in water/rock interaction modelling?

4.2 Task 5 modelling

4.2.1 Scope, objectives and rationale

The principle aim of the Äspö Task 5 modelling exercise is to compare and ultimately integrate hydrogeochemistry and hydrogeology using the input data from the pre-investigation and construction phases. The main objectives were:

- to assess the consistency of groundwater-flow models and hydrogeochemical mixing-reaction models through integration and comparison of hydraulic and hydrogeochemical data obtained before and during tunnel construction, and
- to develop a procedure for integration of hydrological and hydrogeochemical information which could be used for disposal site assessments.

The rationale behind these modelling exercises was based on the following:

- groundwater flow and chemistry are important for conditions for the safety and performance assessment of a deep geological disposal of radioactive waste,
- if groundwater flow and chemistry are integrated properly, it should give better confidence in the description of present and future conditions at a potential repository candidate site, and
- the modelling approaches used in Task 5, if considered successful, could be used for any future repository site investigations, especially in a fractured crystalline rock environment.

4.2.2 Performance measures

The general method of addressing the Task 5 modelling objectives was to compare the outcome of two independent modelling approaches: a) hydrodynamic approach whereupon the groundwater compositions are predicted, and b) hydrogeochemical approach whereupon the groundwater compositions are measured. In order to facilitate comparison, a series of control points were identified along the tunnel. These locations mostly related to the intersection of the tunnel with hydraulically active fracture zones and formed part of the long-term monitoring programme where both hydraulic and hydrochemical parameters were routinely measured. The location of these control points used in Task 5 has been already described in Section 3.3.4 and illustrated in *Figure 3-7*. Based on these tunnel locations, a series of measures were identified to check the performance of the models. These performance measures are:

- the nature of the groundwater flow pattern through the bedrock to the tunnel control points
- the advective groundwater travel time distribution to the control points, and
- the nature of the groundwater chemical evolution to explain the results at each control point.

Two different modelling aims were specified: a) tunnel section 0-2900 m was chosen for model calibration and all pre-construction and construction data were made available, and b) tunnel section 2900-3600 m was chosen for model prediction where only the pre-investigation input data were made available; the objective was to predict the construction phase disturbance.

4.3 Hydrodynamic modelling approaches applied by the modelling teams

Most of the Task 5 groups modelled only the Hydraulic Conductor Domains (HCDs). Models including both HCDs and Hydraulic Rock mass Domains (HRDs), were used by ANDRA/ANTEA, CRIEPI, JNC/Golder, Posiva/VTT and SKB/CFE/Intera. The continuum approach was used for the HCDs and HRDs but one group used Channel Network for HCDs (ANDRA/ITASCA) and one group assumed constant properties for the HCDs and modelled the HRDs as a Discrete Fracture Network (JNC/Golder).

Dispersion and diffusion were considered by some modelling teams but sorption/desorption were not considered relevant; matrix diffusion was considered by one team (Posiva/VTT).

In Table 4-1 the modelling approaches are summarised.

Table 4-1: Modelling approaches (not the capability of the numerical codes) used by the different groups.
(Note: JNC/Golder: X(1), X(2) and X(3) represent different model stages; ^{1}: Fluid, variable density-refers to particle transport, not flow and head calculations. Posiva/VTT: X(1) and X(2) represent different model cases; ^{2}: Assigned value is dependent of depth. SKB/CFE/Intera: (1) and (2) represent different model cases). (X): Partly takes account for the model characteristics mentioned.

Model characteristics	ANDRA / ANTEA	ANDRA / CEA	ANDRA / ITASCA	BMWi / BGR	CRIEPI	ENRESA / UDC	JNC / GOLDER	POSIVA / VTT	SKB/ CFE/ Intera (1)	SKB/ CFE/ Intera (2)
Modelling approach:										
Finite element	X	X	X	X	X	X	X	X		
Finite difference (Finite volume)									X	X
Fracture network							X			(X)
Channel network			X							
Continuum	X	X	(X)	X	X	X		X	X	X
Hydrodynamic:										
- Transient	X	X	X	X	X	X	X	X		
- Steady state–stepwise w. updated b.c.									X	X
Transport: (processes included)										
- Advection	X	X	X	X	X	X	X(1,2,3)	X	X	X
- Dispersion+Diffusion		X	X	X	X	X		X	X	X
- Macro dispersion due to K distribution							X (3)		X	X
- Matrix diffusion										
Transport: (flow paths and concentration)								X		
- Advection/diffusion equation										
- Adv./diff. equ.for tracking each comp.	X	X		X	X	X	X	X		
- Particle tracking (concentration)									X	X
- Particle tracking (flow paths)			X							
			X		X		X(3)		X	X

Model characteristics	ANDRA / ANTEA	ANDRA / CEA	ANDRA / ITASCA	BMWi / BGR	CRIEPI	ENRESA / UDC	JNC / GOLDER	POSIVA / VTT	SKB/ CFE/ Intera (1)	SKB/ CFE/ Intera (2)
Model size (approx.):										
East-west (m)	3750	2000	2000	2000	2000	2000	2000	3300	1800	1800
North-South (m)	2620	2000	2000	1800	2500	2000	2000	3300	1800	1800
Depth (m)	1500	1000	1000	1000	1000	1000	1000	1500	1000	1000
Geometrical units :										
Hydraulic Conductor Domains (HCDs)	X	X	X	X	X	X	X	X	X	X
Extra features (HCDs) added by group							X			
Hydraulic Rock mass Domains (HCDs)	X				X		X	X	X	X
Spatial assignment properties – HCDs :										
Constant	X	X	X	X		X	X	X^2		
Constant → Continuum (Smearing)					X				X	X
Dual porosity (kinematic + diff. porosity)								(X)		
Internal variability: // and ⊥ to HCD plane	X									
HCD intersections: T specified	X		X			X				
Spatial assignment properties – HRDs:										
Constant	X				X			X		
Stochastic continuum									X	
Fracture network→ Continuum (Smearing)										X
Dual porosity (kinematic + diff. porosity)								X		
Kinematic porosity decrease towards depth								X		
Stochastic Discrete Fracture Network							X			

Model characteristics	ANDRA / ANTEA	ANDRA / CEA	ANDRA / ITASCA	BMWi / BGR	CRIEPI	ENRESA / UDC	JNC / GOLDER	POSIVA / VTT	SKB/ CFE/ Intera (1)	SKB/ CFE/ Intera (2)
Fluid: Variable density = f(salinity)		(X)					(X(1,2))[1]	X		X
Boundary conditions /Top/Land :										
Increased K uppermost cell layers (0-10m)									X	X
Constant flux	X	X			X	X	X			
No flow/ flow after tunnel = f (time)				X						
Water table init. t-step/ inflow near shaft								X		
Flux rate dependent on level of water table			X						X	X
Meteoric water	X	X	X	X	X	X	X	X	X	X
Boundary conditions/Top/Sea :										
Increased conductivity uppermost layer									X	X
Sea-bed "skin"			X				X		X	X
Hydrostatic head	X	X	X	X	X	X	X	X	X	X
Sea salinity								X	X	X
Baltic Sea	X	X	X	X	X	X	X	X(1)	X	X
Inverse modelling results								X(2)		

Model characteristics	ANDRA / ANTEA	ANDRA / CEA	ANDRA / ITASCA	BMWi / BGR	CRIEPI	ENRESA / UDC	JNC / GOLDER	POSIVA / VTT	SKB/ CFE/ Intera (1)	SKB/ CFE/ Intera (2)
Boundary conditions/Sides:										
Hydrostatic head		X	X	X	X	X		X		
Head from regional model – constant	X						X			
Head from regional model – f(time)									X	X
Salinity from regional model – f(time)									X	X
Mixing ratios – constant		X	X	X	X	X	X(1,2)	X(1)		
Mixing ratios – f(time)	X								X	X
Chemical composition derived from obs.							X(3)			
Inverse modelling results								X(2)		
Boundary conditions/Bottom:										
No flow	X	X	X		X	X	X	X		
Hydrostatic head				X						
Head from regional model – f(time)									X	X
Salinity from regional model – f(time)									X	X
Mixing ratios – constant				X				X(1)		
Mixing ratios – f(time)									X	X
Inverse modelling results								X(2)		
Boundary conditions/Tunnel & shafts:										
Specified flow = f(time)	X		X		X		X		X	X
Tunnel ‘skin’ (effect of grouting/geometry)		X				X				
Atmospheric pressure		X						X		
Specified head				X		X				

4.4 Hydrogeochemical modelling approaches applied by the modelling teams

The use of hydrogeochemistry in modelling hydrodynamic flow has normally been restricted to salinity/density input parameters, i.e. physical parameters easily integrated mathematically into the numerical models. A concerted effort therefore was made in Task 5 to expand the quantitative use of hydrogeochemistry. Since existing integrated codes are few, Task 5 provided the opportunity of modifying such models that exist or developing new model approaches. To establish some common ground and provide constraints on the modelling, SKB decided to provide the modelling teams with calculated groundwater end member mixing proportions for each of the control points; these mixing ratios were calculated using the M3 method (see Section 3.4). The modelling teams were also presented with the list of groundwater chemical reactions known to occur at the Äspö site and which may influence the groundwater chemistry (see Section 3.4); the teams were given the option to incorporate these reactions.

Table 4-2 summarises the use of hydrogeochemistry made by the various modelling groups, i.e. groundwater mixing ratios and chemical reactions. All modelling groups used the distributed M3 mixing ratio data set as required; six out of the nine groups addressed the influence of chemical reactions. Note also that some groups (e.g. BMWi/BGR, CRIEPI, JNC/Golders and Posiva/VTT) used other approaches to calculate groundwater mixing ratios, in particular Posiva/VTT and JNC/Golders who presented alternative methods from first principles.

Table 4-2: General summary of the use of hydrochemistry by the different modelling groups

	ANDRA/ ANTEA	**ANDRA/ CEA**	**ANDRA/ ITASCA**	**BMWi//BGR**	**CRIEPI**	**ENRESA/ UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/ Intera**
Use of M3-calculated groundwater mixing ratios	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Origin of M3^1 (Mixing and Massbalance Model)
Alternatively-calculated groundwater mixing ratios	No	No	No	Yes, recalulated using PHREEQC with Cl, Na and ^{18}O acting as conservative tracers.	Yes, using the FEGM/FERM coupled code for groundwater flow and solute transport	No	Yes, Principal Component Analysis (PCA). Model uses a chemometric algorithm^2	Yes, inverse geochemical modelling using PHREEQC-2	No
Influence of chemical reactions during groundwater mixing	Not considered	Not considered	Yes, using the FLO code based on principal components and assuming thermodynamic equilibrium	Yes, geochemical thermodynamic equilibrium modelling using PHREEQC	Yes, geochemical thermodynamic equilibrium modelling using PHREEQE	Not considered	Yes, qualitative indication of reactions using PCA.	Yes, inverse geochemical modelling using PHREEQC-2^3	Yes, qualitative indication of reactions using M3 and Voxel 3D interpolation.
<u>Chemical reactions of importance</u>	Not considered	Not considered	Yes considered	Yes, considered	Yes, considered	Not considered	Yes, considered	Yes, considered	Yes considered
- HCO$_3$ production caused by decomposition of organic material in meteoric water			Not considered	Significant	Significant		Significant; suggested microbial processes	Significant	Significant

	ANDRA/ ANTEA	**ANDRA/ CEA**	**ANDRA/ ITASCA**	**BMWi//BGR**	**CRIEPI**	**ENRESA/ UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/ Intera**
- Consumption of dissolved oxygen in meteoric water by pyrite oxidation			Not considered	Significant	Not significant		Indicated	Yes, dissolution of goethite under undisturbed conditions	Both yes and no depending on site location
- Precipitation and dissolution of calcite			Significant	Significant	Not significant		Not indicated	Significant	Significant
- Cation exchange by clay minerals			Not considered	Significant; loss of K, gain of Mg and Na	Significant		Significant; suggested exchange of Ca/Na for Mg/K	Significant; suggested exchange of Na for Ca; Na for Mg; Na for Fe	Both yes and no depending on site location
- Oxidation-reduction between HS^- and SO_4^{2-}			Not considered	Significant	Not significant		Not indicated	Significant; pyrite precipitation	Both yes and no depending on site location

[1] = Laaksoharju et al. (1999)
[2] = Cave and Wragg (1997)
[3] = Pitkänen et al. (1999)

4.4 Integration of hydrodynamics and hydrogeochemistry

The principle aim of Task 5 was to integrate hydrogeochemistry with hydrogeology. To facilitate integration all groups used the SKB M3 hydrochemical end member mixing ratios as input to the hydrodynamic modelling exercise (e.g. initial and boundary conditions) and all models used the control point M3 calculated hydrochemical mixing ratios to compare modelled simulations (e.g. for calibration purposes). In an attempt to formalise individual modelling approaches, one of the requirements from the modelling teams was to provide a flow chart showing how they intended (and actually accomplished) to integrate hydrogeochemical data into their respective hydrodynamic models. As an example, the intended approach of SKB/CFE was distributed to all participants (*Fig. 4-3*); four out of the nine groups responded.

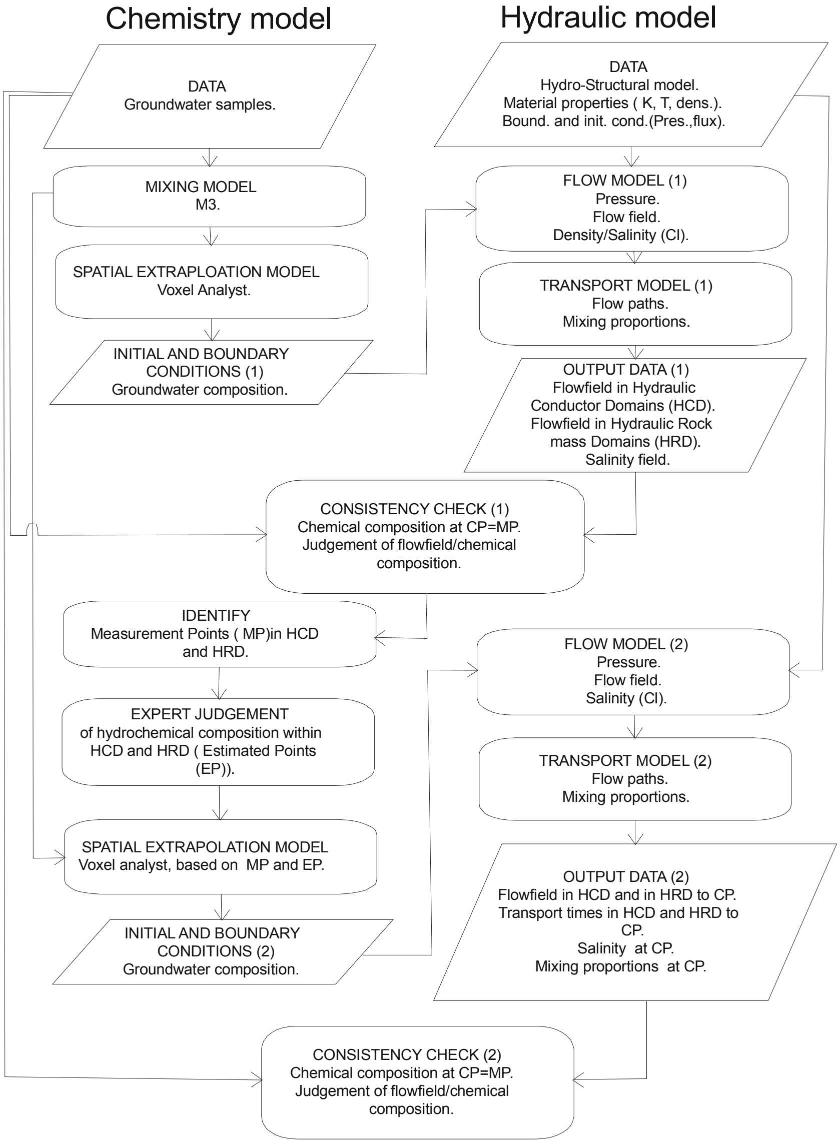


Figure 4-3. *The SKB/CFE integrated approach (initial outline) (Svensson et al., 2002).*

The SKB/CFE integrated approach *(Fig. 4-3)* emphasised that it should be performed in two steps with a consistency check as the final event in both steps. The approach of Posiva/VTT was largely similar to that of SKB/CFE (*Fig. 4-4*). In both cases, in common with other teams, the consistency check compared the measured chemical composition (or mixing ratios) at each control point with the chemical composition (or mixing ratios) from the hydrodynamic model. Modelling of the flow field incorporated input of flow, pressure, salinity/density and groundwater end member types.

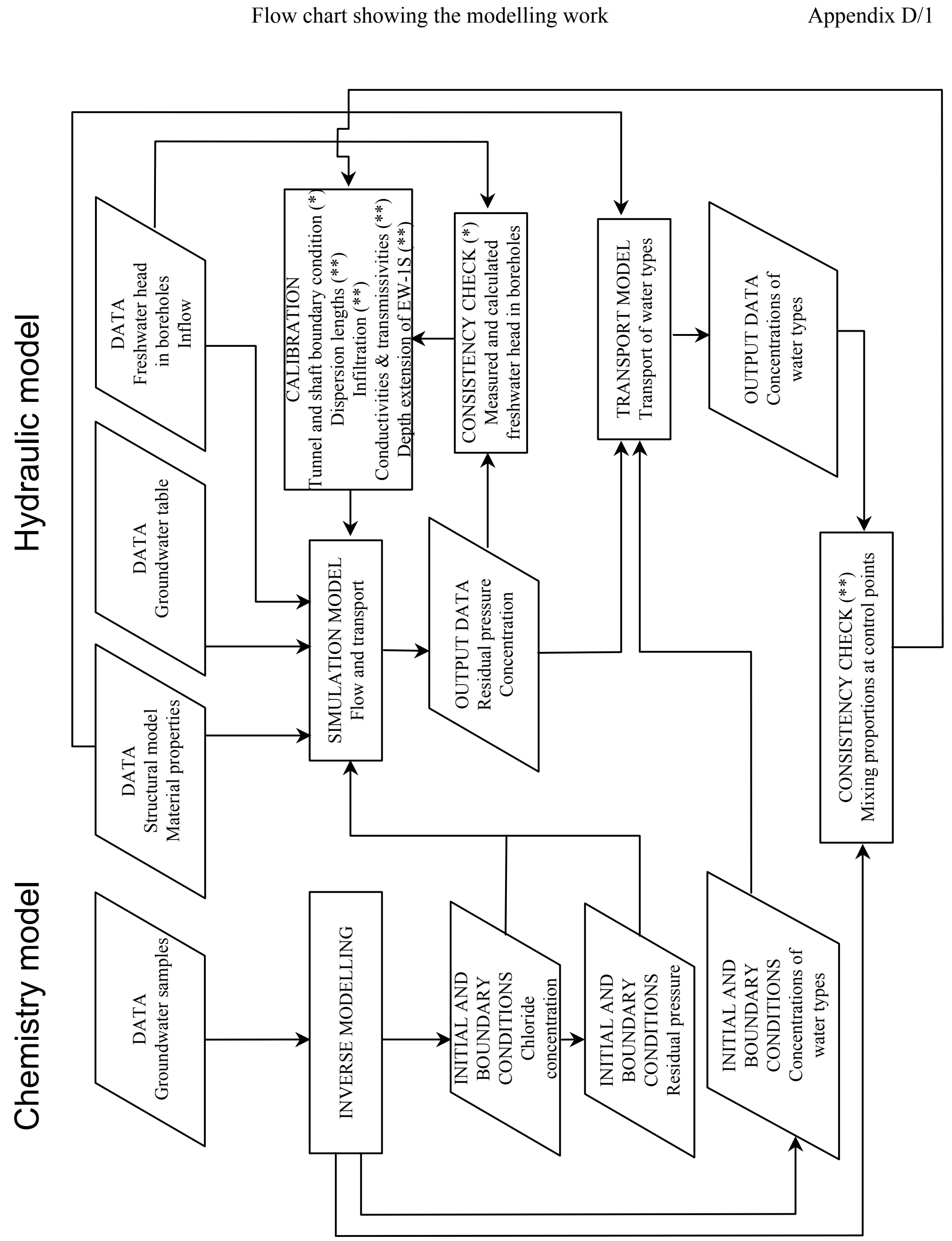


Figure 4-4. *Flow chart of the integrated modelling approach carried out by Posiva/VTT (Luukkonen and Kattilakoski, 2002).*

JNC/Golder constructed a flow model which was then run with the initial boundary condition groundwater chemistry (mixing proportions). Differences between measured and modelled hydrochemistry were used then to calibrate the hydrodynamic model. Furthermore, they considered the chemistry as pure mixing in the particle tracking carried out. The general procedure for integration of the hydrological and hydrochemical information used by Golder/JNC was carried out in stages which were summarised as follows:

1. Modelling with calibration of only hydrogeological data – prediction of hydrogeochemistry.
    - Develop a regional model of the site including only the large scale features
    - Develop a conceptual model for the background fractures. For a discrete fracture network idealisation this included the orientation, size, intensity, and transmissivity of the non-regional features. For porous medium models this would be the equivalent block transmissivities.
    - Develop boundary conditions for the modelled region.
    - Create a finite element model including the major features, background features, and boundary conditions. Calibrate this model to the measured head distribution by varying the fracture properties and boundary conditions.
    - Use this calibrated model to predict chemistry distributions.
2. Modelling with calibration of hydrogeological and hydrogeochemical data.
    - Evaluate the predicted chemsitry versus measurements to refine/modify modelling conepts , geometry and properties.
    - Calibrate this model to the measured chemistry and head distribution by varying the fracture properties and boundary conditions.

Since this staged approach is very general, it was considered applicable to other potential repository sites. The staging was advantageous because it necessitated constructing a good geology based discrete fracture network model of the site prior to calibration. Without such a structure for the discrete fracture network, the problem would be poorly constrained and the calibration non-unique. A unique calibration likely cannot be obtained in practice, but the staged approach should enable the dominant features to be well replicated.

The type of chemical reactions that took place during groundwater mixing was addressed by six of the nine groups, with a more quantitative evaluation by four groups (Section 4.4; Table 4-2). BMWi/BGR emphasised the importance of chemical equilibrium reaction processes (particularly in the pre-investigation phase) together with mixing processes (dominating the construction phase) to explain the groundwater compositions at Äspö. The hydrodynamic modelling approach simulated flow and solute transport and the PHREEQC code was used to model the reaction chemistry. Both modelling approaches were carried out in two different steps that had to be combined in succession (*Fig. 4-5*). The transport or mixing model provided the water compositions at the control points that were compared to the measured values. Possible deviations, suggesting chemical reactions, were then evaluated by chemical methods. Finally, using the time-series measured groundwater compositions a hydrogeochemical model was established which was used to simulate the control point compositions.

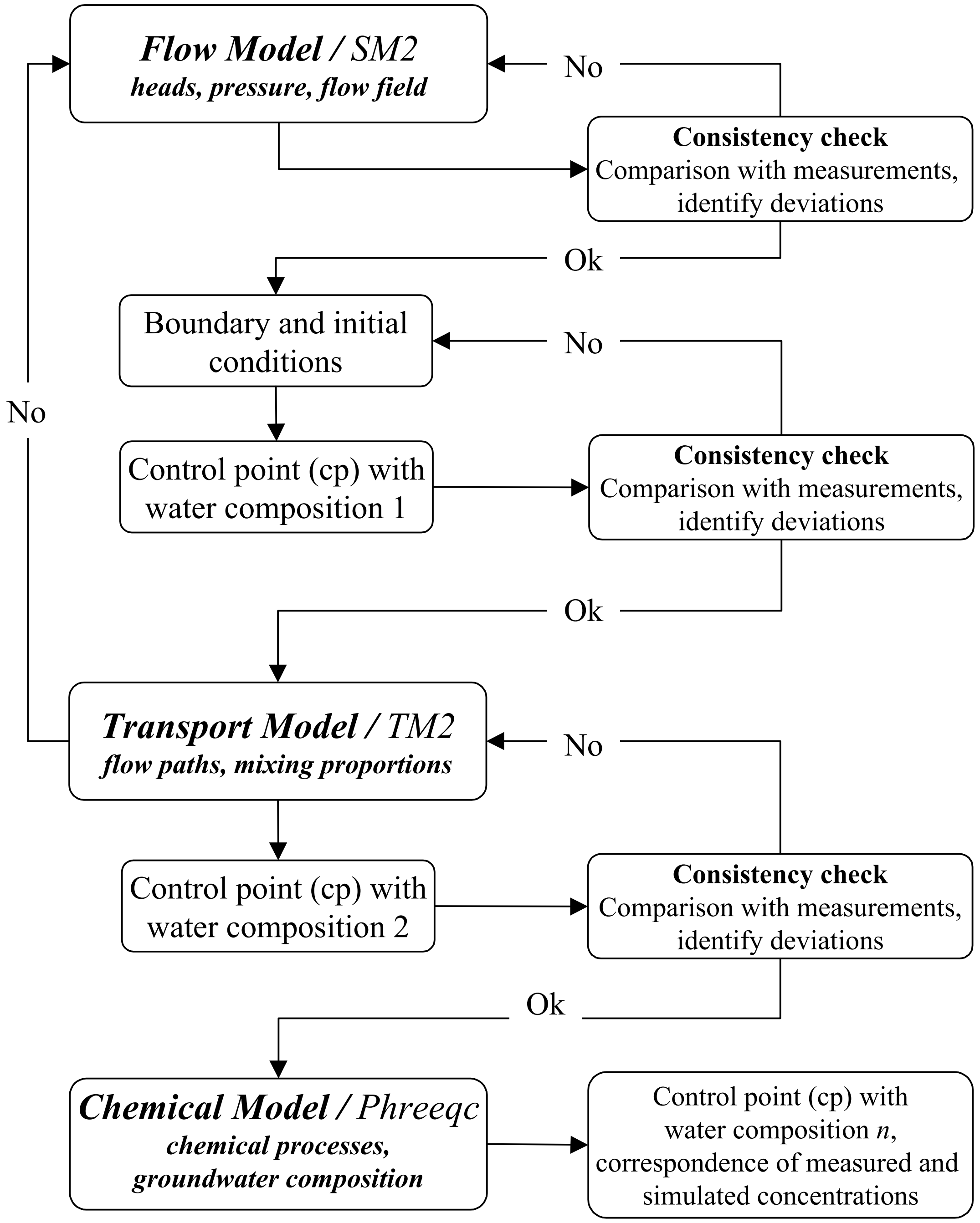


Figure 4-5. *Flow chart of the integrated modelling approach carried out by BMWi/BGR (Liedtke and Klennert, 2002).*

CRIEPI combined groundwater flow modelling with solute transport (constrained to conservative species, Cl and $\delta^{18}O$) and chemical reaction modelling using PHREEQE (*Fig. 4-6*). The modelling follows mainly three paths, geochemical, groundwater flow and transport modelling. The consistency checks are made on several levels and it is the groundwater flow model that is the main link between the paths.

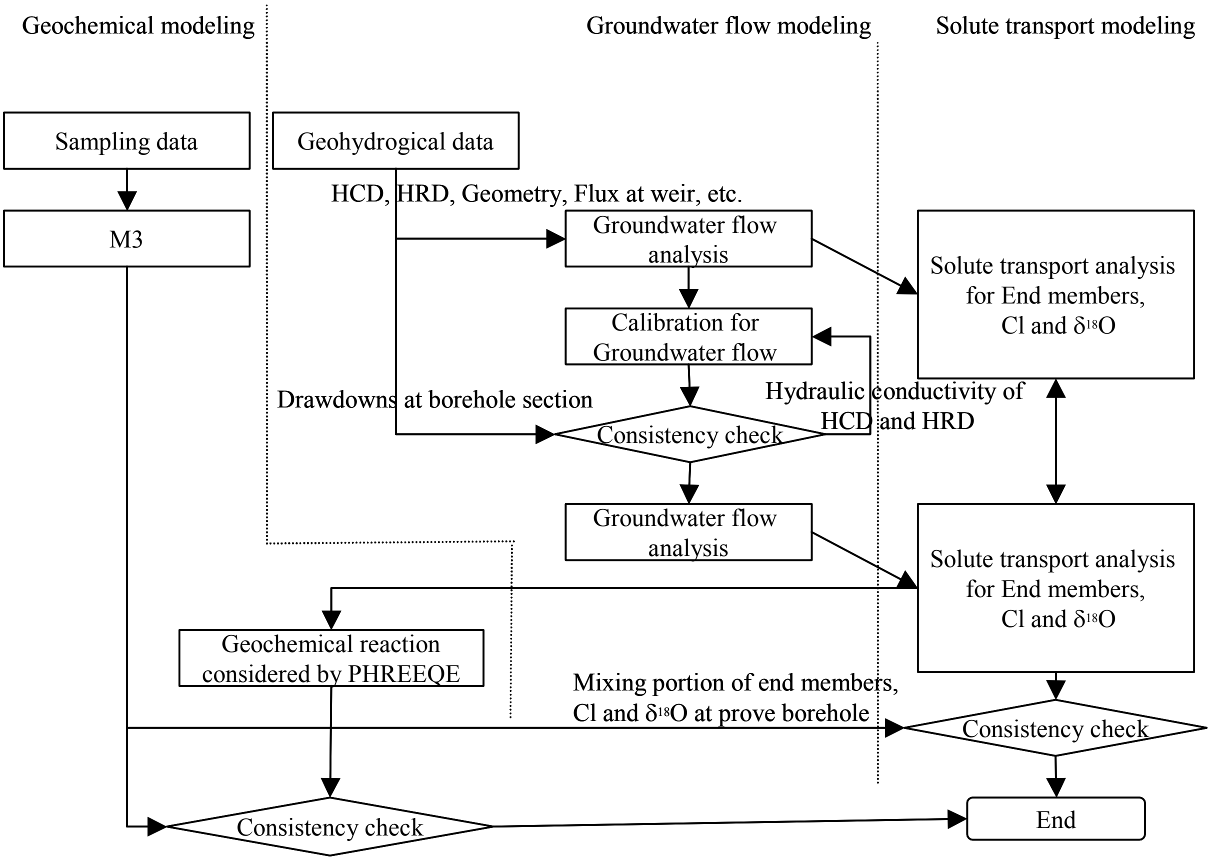


Figure 4-6. *Flow chart of the integrated modelling approach carried out by CRIEPI (Hasegawa et al., 2002).*

ENRESA, ANDRA/CEA and ANDRA/ANTEA all restricted the use of hydrochemistry to initial and boundary condition input and flow model calibration. All these groups stressed the importance of sensitivity analysis to understand the influence of different concepts and modelling applications on the flowfield and the transport of solutes.

Integration of hydrogeology and hydrochemistry using coupled transport/hydrogeochemical simulations were performed by ANDRA/ITASCA and ENRESA/UDC. ANDRA/ITASCA performed these in a limited region of the hydrodynamic model. The modelling approach initially used the groundwater mixing ratios to better calibrate the hydrodynamic model; the coupled geochemical model assumed thermodynamic equilibrium conditions and only one potential chemical reaction was considered, that of carbonate dissolution/precipitation.

As indicated above, ENRESA/UDC did not hydrogeochemically model the influence of chemical reactions during groundwater mixing as part of the Task 5 exercise. However, outside the framework of the project they carried out numerical simulations on the Redox Zone, which intersects the access tunnel at 70 m depth (*Banwart et al., 1999*). The simulations were carried out using the CORE^{2D} finite element code which solves groundwater flow, heat transport and multi-component reactive solute transport under variably saturated conditions (*Molinero et al., 2002*; Appendix 5). The model reproduces the measured hydrogeological response, as well as the observed concentrations of most dissolved species both before and after tunnel construction. The model was able to reproduce the observed behaviour of most dissolved species and showed that discrepancies could be largely explained by microbially-mediated processes (see section 5.6.5).

In addition to their formal Task 5 integrated approach detailed in Figure 4-6, CRIEPI expanded on some earlier relevant work related to helium (^{4}He) contents in groundwaters sampled during two tunnel campaigns in 1995 and 1997. Although the localities sampled did not correspond to the Task 5 control points, they were considered to be useful generally in helping to understand the flow system at Äspö.

The consistency between the chemical properties of the collected samples and groundwater flow modelling were checked by performing numerical calculations. In practice it was relatively easy to simulate the dissolved helium concentrations since:

- the boundary conditions are quite simple to evaluate the distribution of helium; for example, the source of ^{4}He is a constant rate production from the rock and therefore the concentration of helium will be an atmospheric equilibrium concentration at the ground surface
- the flow field can be simply determined; for example, since the helium concentration depends on the residence time, it will be lower following shorter residence times and subsequently higher following longer residence times
- the helium concentration will tend to increase with increasing depth as flow become more stagnant.

The simulated helium concentrations generally were found to be in good agreement with the measured concentrations. Since the measured and simulated results reflect the hydraulic properties of the HCDs, it is considered a potentially useful method to verify the hydrogeological model.

5 Modelling: Application and results

5.1 General

This Chapter summarises the results in the modelling reports and presents the conclusions reached by the different groups. In section 5.2 the M3 hydrochemical modelling is presented in reasonable detail since it provided a common basis for the hydrodynamic modelling tasks. Section 5.3 summarises the available data and how it was used. The hydrogeological modelling is summarised in section 5.4 with some compilation characteristics and results of the different models. The hydrodynamic simulations of the M3 mixing ratios are found in section 5.5 and the influence of chemical reactions on the groundwater chemistry during mixing in section 5.6. Alternative hydrogeochemical approaches are summarised in section 5.7.

All the results presented in this chapter are a compilation of model applications within Task 5, together with some selected illustrations of modelling results and some brief comments. Detailed information is found in the following list of reports which are accompanied by the acronyms used in this report and the main authors: *Wendling (2000)*(ANDRA/ANTEA), *Grenier and Benet (2000)* (ANDRA/CEA), *Billaux and Paris (2001)* (ANDRA/ITASCA), *Liedtke and Klennert (2001)* (BMWi/BGR), *Hasegawa et al. (2001)* (CRIEPI), *Molinero et al (2001)* (ENRESA/UDC), *Dershowitz et al. (1998,2000)* (JNC/GOLDER), *Luukkonen and Kattilakoski, (2001)* (Posiva/VTT), *Svensson et al. (2002)* (SKB/CFE). The modelling work has also been reviewed by *Bath and Jackson (2002).*

5.2 Hydrochemical modelling (M3)

This section includes the selection of the reference (or end member) waters, testing the suitability of the M3 model, how the M3 modelling approach has been used to trace the hydrochemical changes during tunnel construction, and finally to compare the measured and calculated groundwater mixing proportions at selected control points along the tunnel length.

5.2.1 General

Modelling, based mainly on the M3 approach, constituted the active hydrogeochemical contribution to Task 5 by SKB and is treated separately in this section because of its overall importance to the Task 5 modelling. It has a two-fold contribution:

- to fulfill SKB's contribution to the main Task 5 objective of integrating hydrogeochemistry with a hydrodynamic groundwater flow model, and
- to provide calculated groundwater mixing ratios from each control point to the other modelling groups to achieve some common ground for model comparison

The strategy of integrating hydrogeochemistry with hydrogeology has been outlined above in section 4.5 and M3 modelling provides the basis for integration. M3 modelling has been used for some time in the SKB hydrogeochemical programme and initially was used to model the Äspö groundwater system in the pre-construction phase and, subsequently during the construction phase *(Laaksoharju, 1999).* The initiation of Task 5 conveniently coincided with a period of continued development of M3, such that much of the background M3 data were already available. Moreover, because of the Task 5 objectives, this modelling exercise also provided an opportunity for further M3 refinement and application.

As a complement to the M3 modelling, use was made of the Voxel Analyst computer code which allowed a 3D interpolation and visualisation of the data on a site scale.

5.2.2 Results

The M3 hydrogeochemical modelling is systematically described and presented in Chapters 4-6 in *Svensson et al. (2002).* The step-wise approach employed in the Task 5 modelling was as follows:

- Selection of reference waters (or end members) using data for the undisturbed system
- Testing the suitability of the M3 model
- Modelling and visualising the changes in groundwater composition due to the tunnel construction (0-2900 m tunnel length)
- Comparison of measured and calculated mixing proportions at selected control points (0-2900 m tunnel length)
- Modelled predictions of mixing ratios at selected control points (2900-3600 m tunnel position) by extrapolation of trends for various water classes
- Comparison of predictions at all control points (0-3600 m tunnel position)

Reference waters and suitability of the M3 model

Using the PCA analysis (see section 3.4) four major reference (or end members) waters were identified: Äspö Brine, Glacial Water, Meteoric Water and Marine Water. These reference waters ensured that most of the groundwater samples plotted within the polygon (*Fig. 5-1*) and could therefore be further modelled using M3. In detail, additional reference water-types could be indicated (e.g. Litorina Sea, Modified Sea water; *Laaksoharju et al., 2000*), but to facilitate the Task 5 hydrodynamic modelling exercise it was decided for simplicity and practical reasons to work with the four major reference waters. Figure 5-1 also addresses the effect from the analytical uncertainties on the position of a sample in the plot and hence the effect on the modelling.

The suitability of the selected model was assessed by comparing the mixing proportions and element contribution for the different reference waters with the measured values for the different chemical species in the groundwater samples (*Fig. 5-2*). If the calculated and the measured values coincided then the chemistry of the sampled groundwater(s) could be explained largely by mixing of the selected reference waters. Contrastingly, a positive deviation (above the ideal mixing line) or a negative deviation (below the ideal mixing line) indicated the influence of chemical reactions during groundwater mixing that either contributed to, or removed chemical species from, the sampled groundwaters. Figure 5-2 shows that mixing mostly explained the distribution of the two conservative tracers (i.e. Cl and ^{18}O) but water/rock interactions played a more dominant role in the distribution of Mg, K, HCO_3 and SO_4.

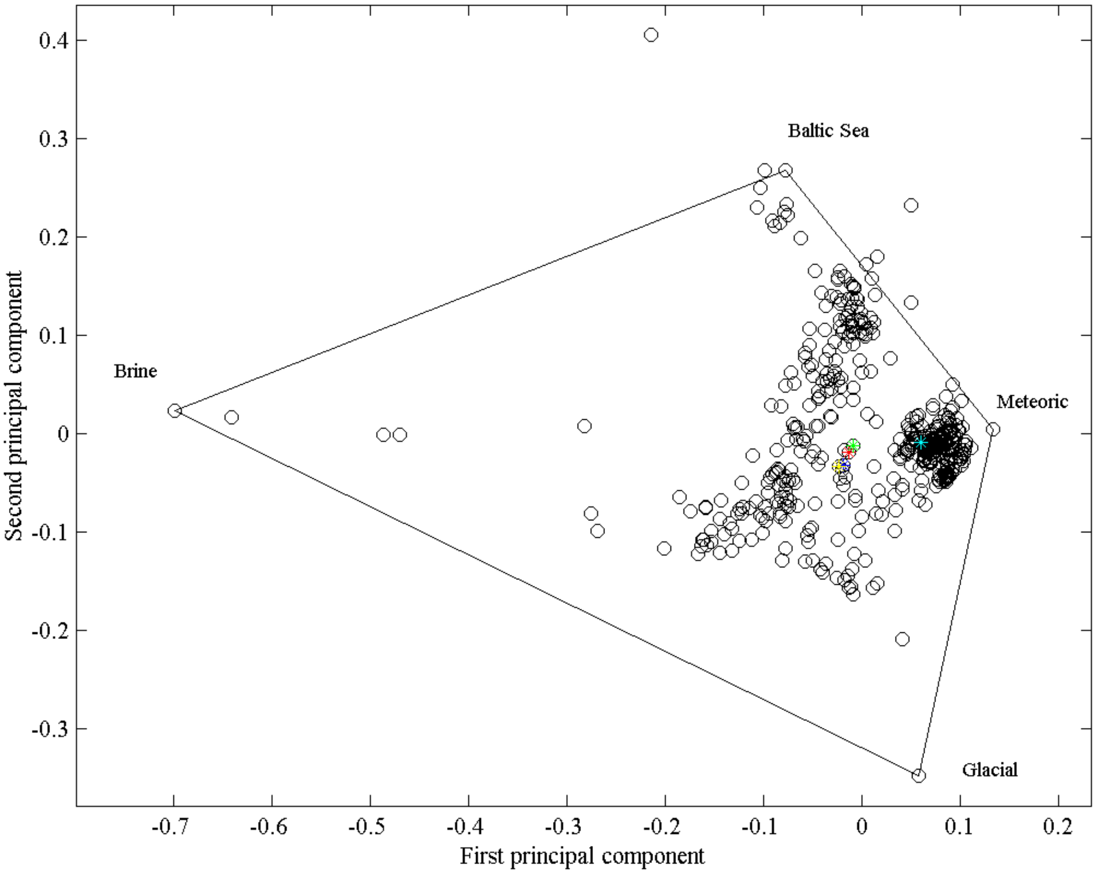


Figure 5-1. The Principal Component plot based on the water conservative tracers Na, K, Ca, Mg, Cl, SO_4, HCO_3, ^3H, δ^2H and $\delta^{18}O$ applied on Task 5 data. The figure also shows the effect from the analytical uncertainties on the position of a sample in the plot and hence the effect on the modelling. Initially the measured components were altered by +5% (blue dot) and by -5% (green dot) from the reported value (red dot) for sample SA1420A. The observed changes are minor. Tritium was then changed from the measured 17TU to 0TU (yellow dot) but keeping the other elements as reported. This mostly changed the position in the PC-plot and changed also the mixing calculations in the following way (the mixing calculations based on the sample where TU was 0 and where TU was 17 are in brackets): Brine +0.02% (13.24%, 13.22%), Glacial +6.10% (22.96%, 16.86%), Meteoric –6.12% (50.57%, 56.69%) and Baltic Sea +0.02% (13,24%, 13.22%). The tests show that the changes in the plot are minor and less than the reported model uncertainty of ±10% and do, therefore, not affect the overall interpretation.

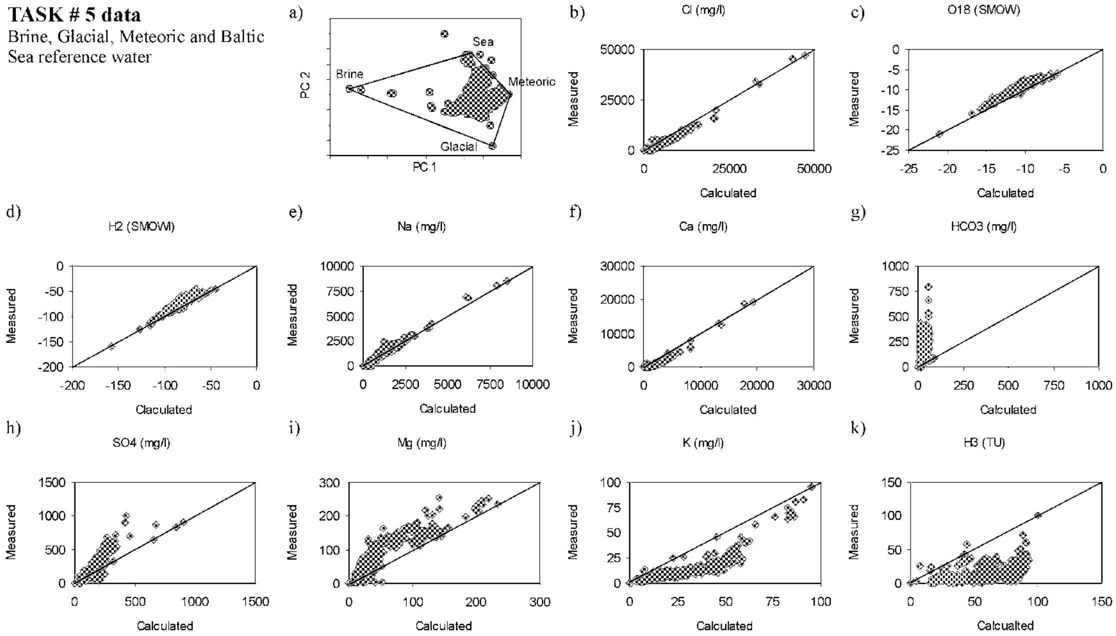


Figure 5-2. The Task 5 groundwater is modelled to be a mixture of Brine, Glacial, Meteoric and Baltic Sea reference waters as shown in the PCA (Fig. 5-2a). The calculated values based on the mixing proportions and the element contribution from reference waters are compared with measured values for different groundwater constituents (Figs.5-2b-k). If the value is on the line the calculated and measured values coincide, if the value is above/under the line there is a deviation between the measured and calculated values. A deviation from the line for the water conservative elements such as Cl, oxygen-18 (^{18}O) and deuterium (^{2}H) indicates scatter in the model. A deviation for a reactive element such as carbonate (HCO_3) can indicate gain (values over the line) or losses (values under the line) associated with chemical reactions (Svensson et al., 2002).

Effects on groundwater chemistry due to tunnel construction

The effects on the groundwater chemistry during tunnel construction were illustrated by two approaches: 1) using the PCA plots, and 2) using the 3D Voxel Analyst visualisation.

PCA plots

The M3 PCA plot is a convenient method of showing time-series changes in groundwater composition. Figure 5-3 shows the simplified compositional changes during tunnel construction by plotting only the first sample in the time series; the tunnel length of approx. 2900 m has been divided into 5 sections for illustration purposes. The changes were quite apparent, for example, the change from meteoric to a Baltic Sea signature along the 500-1000 m tunnel length reflected the fact that the tunnel along this section commenced under land and then continued under the sea.

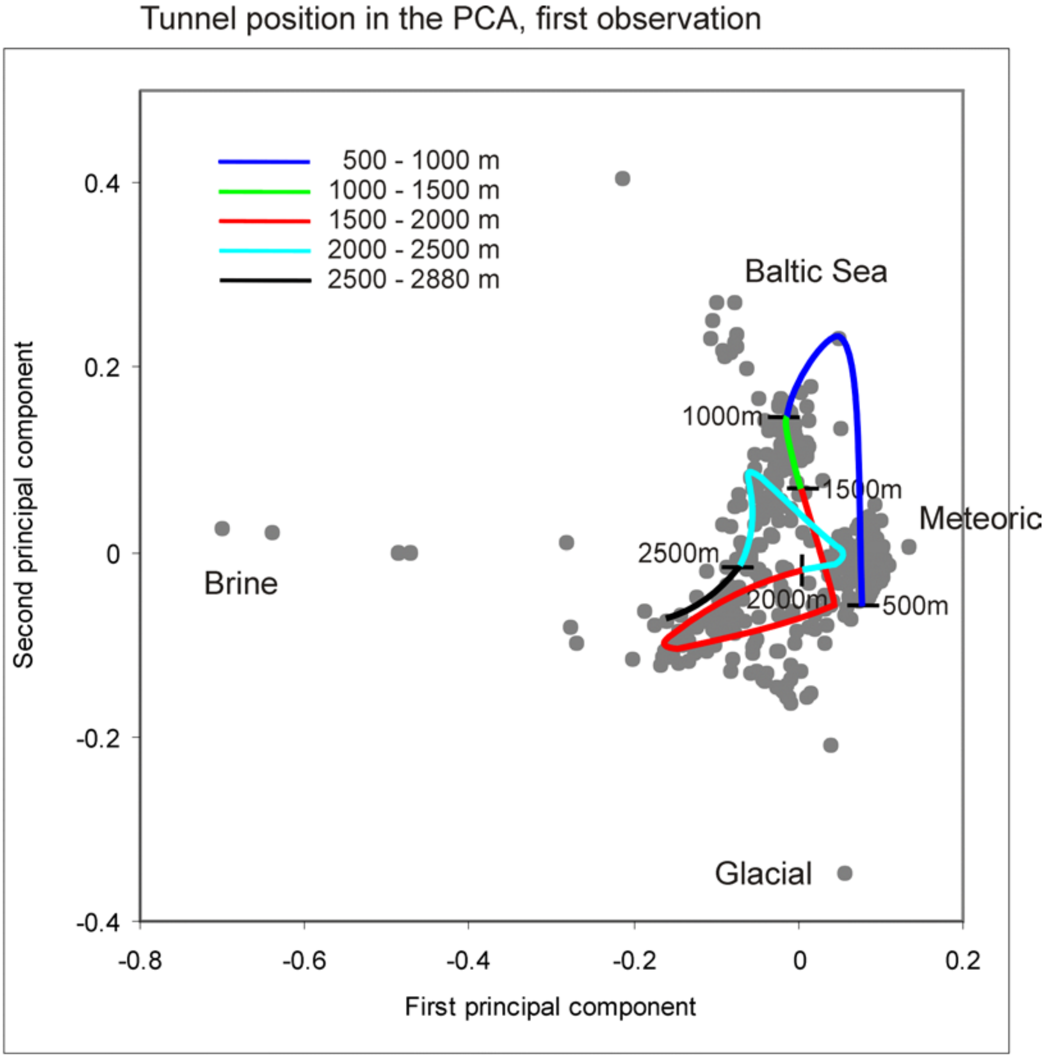


Figure 5-3. *PCA plot shows the general (simplified) changes in groundwater composition in the samples along the tunnel for the first sample in the time-series close behind the advancing tunnel face. The tunnel length and the sampled control points are shown in Figure 3-7. The 500-1000m tunnel section shows that the groundwater changes from Meteoric towards a Marine signature due to the fact that the tunnel starts under the land and continues under the sea. The 1000-2000m tunnel section shows a change from Marine to a Meteoric, Glacial and Äspö Brine signature and then back to a Meteoric signature due to the fact that this section starts under the sea, then continues under Äspö island and ends in the first tunnel spiral. The 2000-2880m section represents the end of the first and the beginning of the second spiral of the tunnel. The water types change from Meteoric to Marine and then towards a more Äspö Brine signature. The reason for the groundwater changes along the tunnel is that the tunnel penetrates different fracture zones located under land, sea and at great depth, which contain different groundwater signatures and hence are reflected in the PC-plot. The variations can only be described by simultaneous changes of all variables as result of mixing and evolution of the water. Non-systematic changes such as analytical errors in some variables do not significantly move the position of the points in the PC- plot (Svensson et al., 2002).*

Of course hydrogeochemical changes were also expected to occur within any one time-series sampling, which may extend over period of months and years, and this was taken into consideration by *Svensson et al. (2002)* in their interpretation. The general trend was that the sampled groundwaters became increasingly mixed with time, a trend also observed from the tunnel data as a whole. It was clear that groundwater changes along the tunnel were the result of the tunnel intercepting vertical to sub-vertical water-conducting fractures of varying strike and geographic location, leading to the mixing of groundwaters of different origins from varying depths in the bedrock.

3D Voxel Visualisation

Based on the measured values of the conservative tracers Cl and ^{18}O and the M3 modelled mixing ratios, representing the pre-investigation and post-construction phases, a series of 3D visualisations were produced to illustrate the extrapolated changes in groundwater chemistry during tunnel construction. As an example, *Figures 5-4* and *5-5* compare, along a 650 m deep horizontal plane, the change in the mixing proportions of the four reference waters during tunnel construction between 1987 and 1996. The effect of the construction, specifically adjacent to the access tunnel and spiral sections, showed a decrease of Baltic Sea signature, marked increase in the Meteoric and Glacial signatures, and a more minor increase in the Äspö Brine signature.

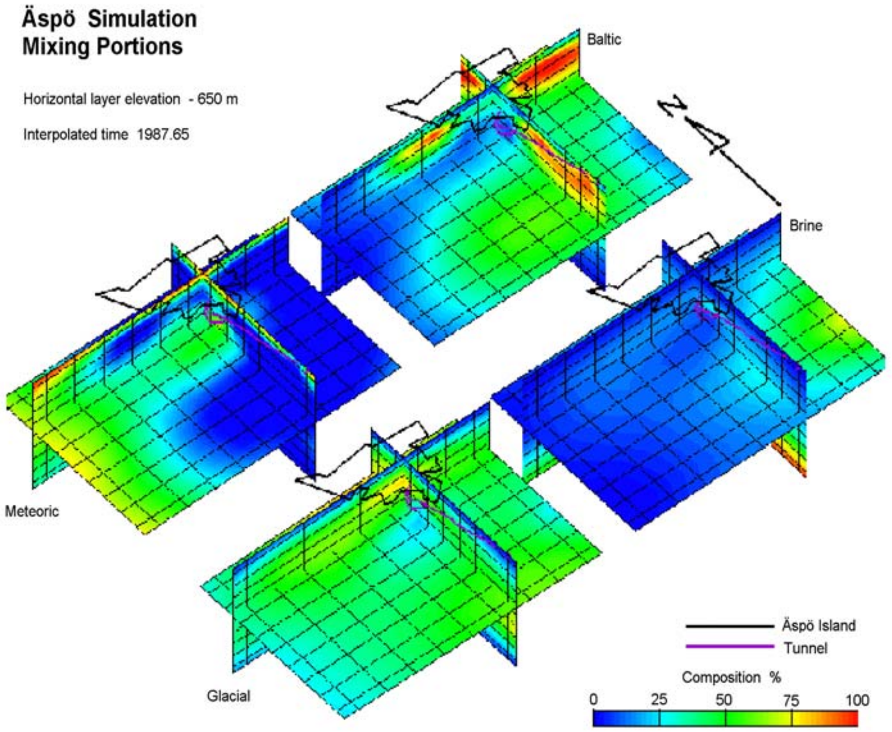


Figure 5-4. *The result of the interpolation of M3 mixing portion calculations (Composition %) for Meteoric, Glacial, Baltic and Äspö Brine waters prior to the Äspö HRL tunnel construction (1987). The contour of Äspö island and the planned extension of the HRL tunnel are shown). The horizontal cutting plane is at –650m depth (Svensson et al., 2002).*

Taking all the plots into consideration (*Figs. 4-3 to 4-7* in *Svensson et al. (2002)),* the influence of tunnel construction resulted in a drawdown towards the tunnel of surface to near-surface Meteoric and Baltic Sea waters, and upconing of Glacial and Äspö Brine waters from depth. Svensson et al. (op. cit.) also presented 3D visualisations of the undisturbed (i.e. pre-construction) reference water mixing proportions along the major water-conducting fracture zones: NE-1, NE-2, NE-3, EW-3 and NNW-4; the illustrated cutting plane was that defined by *Rhén et al. (1997a)* with a depth extension of 1500 m.

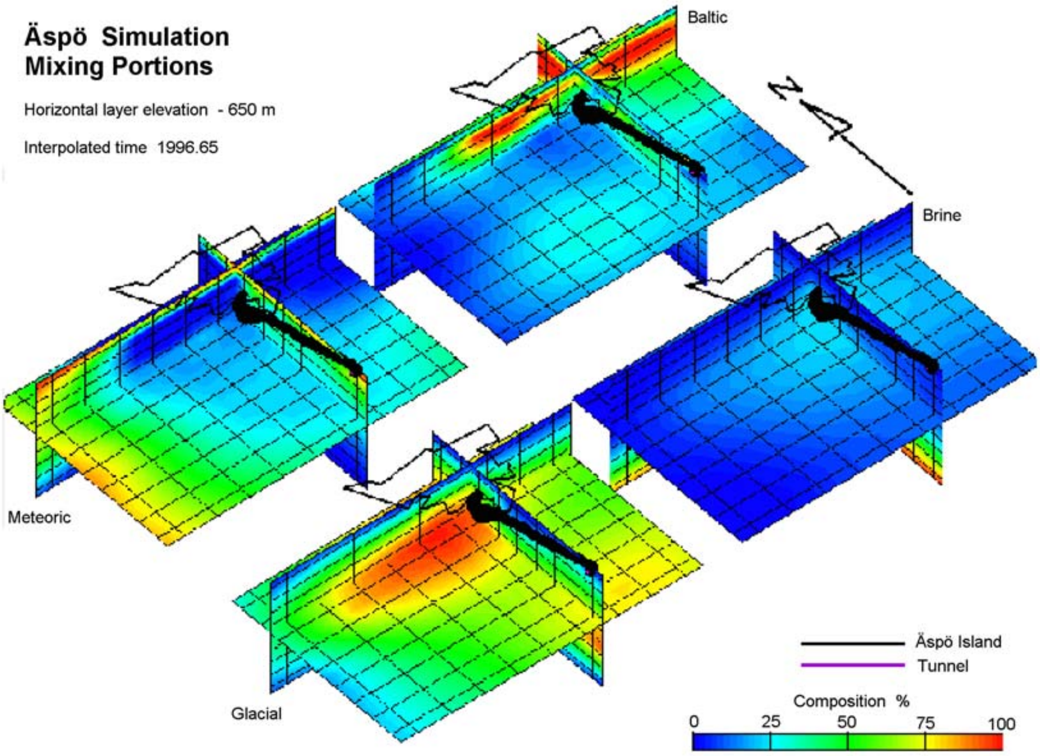


Figure 5-5. *The result of the interpolation of M3 mixing portion calculations (Composition %) for Meteoric, Glacial, Baltic and Äspö Brine waters after the Äspö HRL tunnel construction (1996). The contour of Äspö island and the extension of the HRL tunnel are shown. The horizontal cutting plane is at –650m depth (Svensson et al., 2002).*

Comparison of measured and calculated mixing proportions at selected control points (0-2900 m tunnel length)

With the four major reference waters chosen, the mixing ratios calculated for each control point, the degree of influence of chemical reactions on the groundwater chemistry during mixing indicated, and a good idea of the hydrogeochemical evolution prior to, and subsequent to tunnel construction, the next stage was to compare the measured and calculated mixing proportions at the selected control points in the tunnel.

Svensson et al. (2002) applied various tests on their model approach to determine the potential influence of different parameters on the integrity of the control point groundwater mixing proportions. For example:

- Could changes in groundwater mixing proportions be related to the geometry of the Äspö site (e.g. depth and position of control points etc.)?
- Could changes in groundwater mixing proportions be related to the hydraulic parameters active at the control points (e.g. transmissivity and hydraulic conductivity)?

The tests showed no clear trends that indicated any influence of the geometry of the Äspö site on changes in mixing proportions, and likewise there was no correlation between the hydraulic parameters and groundwater chemistry. The transmissivity and hydraulic conductivity parameters seemed to be control point specific, while the hydrochemical parameters appeared to reflect mixing processes taking place in the larger, surrounding bedrock domain.

A 'Groundwater Calculation Model' was subsequently constructed, an empirical model to predict future changes on the basis of extrapolation using the initial control point values and values at a later time at the site. The basis of this model was to use the mixing proportion of the first time-series sample collected at any one sampling point to predict the last sample collected which is the measured value reported in the data sets. By comparing measured with the predicted values would support or otherwise the potential use/accuracy of the model. It was emphasised that this represented a simplistic approach to modelling the expected short-term groundwater changes and only hydrodynamic models coupled with geology should be used for long-term extrapolation. The input data represented tunnel length 0-2900m to conform with the initial Task 5 aim of using these data for model calibration.

The approach consisted of the following steps:

1. Using the PCA plots the groundwaters were divided into classes (i.e. reference waters) where the dominating mixing proportion in the first time-series groundwater sample determines its class.
2. The changes in mixing proportions between the first and last time-series groundwater samples were calculated by dividing the mixing proportion changes by the number of years to obtain an annual change for each class of water (using data from control points along tunnel section <2900m).
3. To facilitate comparison between the first and last time-series at <2900m, the data were normalised.
4. The mean mixing change per year was calculated.
5. This change was used to add or remove mixing proportions from the first sample in the time-series at >2900m.
6. The predicted mixing water composition was compared with the measured values, i.e. the last time-series groundwater composition.

As a word of caution in evaluating the predicted values *Svensson et al. (2002)* noted that the groundwater chemistry could change during sampling, for example a variation of up to 2000 mg/L Cl in some cases was reported.

The first test of the model was carried out using all the time-series groundwater mixing proportion data representing the regional (Äspö Site) and local (Äspö Island) scales. The tests showed that there was little difference in the predicted values if the regional or site scale models were used to modify the calculated mixing proportions of the first time-series samples (i.e. step 5 above).

Using only the Task 5 data, a summary of the predicted vs measured values is given in Table 5-1. The table shows that the average difference in mixing proportions between measured and predicted for the four main classes was less than 2%. For the major chemical species some were over-predicted (positive values) and others under-predicted (negative values). These deviations were considered as falling within acceptable ranges *(Svensson et al., 2002).*

For tunnel length 0-2900 m the measured vs predicted values were compared using the Voxel Analyst program. Selected input properties included: conservative species Cl and $\delta^{18}O$, reactive species HCO_3 and mixing proportions for Meteoric Water. Comparisons showed that for Cl, $\delta^{18}O$ and Meteoric Water there was reasonable agreement; less so for HCO_3. The deviations were considered to be less than the known uncertainties from natural variation, sampling uncertainties and modelling variations.

Table 5-1: Comparison between average differences in measured vs predicted values for mixing proportion calculations (4 water classes) and major chemical species. (Calculations based on all Task 5 time-series data).

Water Class	**Average Difference**
Äspö Brine	1.2%
Glacial	-0.9%
Meteoric	-0.1%
Baltic Sea	-0.3%
Chemical Species	
Na (mg/L)	-91
K (mg/L)	18
Ca (mg/L)	1356
Mg(mg/L)	-31
CO_3 (mg/L)	-128
Cl (mg/L)	2199
SO_4 (mg/L)	-99
D (‰)	-8
^{18}O (‰)	-1

Comparison of measured and calculated mixing proportions at selected control points (2900-3600 m tunnel length)

The second Task 5 aim, centred along tunnel length 2900-3600 m, was concerned with model prediction at the control points where only the pre-investigation input data were made available; the objective was to predict the construction phase disturbance. Using the predictive approach (linear trend), calibrated and tested as described above, the M3 predictions and Voxel interpolations are tabulated in Table 5-2. The approach was just considered to be possibly be valid for short term predictions.

Table 5-2: The results of the Voxel interpolation (Voxel) and M3 predictions (M3) are listed for each control point >2900m and are compared with the measured data (given data) for Cl, ^{18}O and mixing portions for Meteoric Water, Baltic Sea Water, Äspö Brine and Glacial Water.

ID code	Elevation	Cl Measured	Cl Voxel	Cl M3	^{18}O Measured	^{18}O Voxel	^{18}O M3
KAS03	-566.3	4637	6000-7000	6000-7000	-13.6	<-13	<-13
KAS07	-465.0	5960	5000-6000	8000-9000	-11.2	<-11	-11
KA3005A	-402.2	4870	7000-8000	8000-9000	-9.7	-10	<-10
KA3005A	-402.8	5400			-10		
KA3005A	-403.4	4880			-10		
KA3110A	-416.0	3940	6000-7000	8000-9000	-9.2	-10	<-10
KA3110A	-416.0	3390			-7.7		
KA3385A	-447.5	6650	6000-7000	8000-9000	-10.4	-11	<-10
KA3385A	-448.8	6630			-10.1		
KA3385A	-448.8	6710			-10.5		

ID code	Elevation	Meteoric Measured	Meteoric Voxel	Meteoric M3	Baltic Sea Measured	Baltic Voxel	Baltic M3
KAS03	-566.3	28%	10-20%	10-20%	12%	20-30%	20-30%
KAS07	-465.0	39%	30-40%	30%	17%	20-30%	20-30%
KA3005A	-402.2	53%	20-30%	20-30%	19%	30-40%	30-40%
KA3005A	-402.8	52%			16%		
KA3005A	-403.4	54%			21%		
KA3110A	-416.0	48%	20-30%	30-40%	35%	30-40%	30-40%
KA3110A	-416.0	47%			43%		
KA3385A	-447.5	37%	30-40%	30-40%	19%	20-30%	20-30%
KA3385A	-448.8	42%			18%		
KA3385A	-448.8	36%			19%		

ID code	Elevation	Brine Measured	Brine Voxel	Brine M3	Glacial Measured	Glacial Voxel	Glacial M3
KAS03	-566.3	12%	10-20%	10-20%	47%	40-50%	40-50%
KAS07	-465.0	17%	10-20%	20-30%	27%	20-30%	30%
KA3005A	-402.2	14%	10-20%	20-30%	14%	20-30%	20-30%
KA3005A	-402.8	16%			17%		
KA3005A	-403.4	13%			13%		
KA3110A	-416.0	9%	10-20%	20-30%	9%	20-30%	20-30%
KA3110A	-416.0	5%			5%		
KA3385A	-447.5	19%	10-20%	20-30%	25%	20-30%	30%
KA3385A	-448.8	18%			21%		
KA3385A	-448.8	19%			27%		

From Table 5-2 the following general conclusions were made by *Svensson et al. (2002):*

- The M3 values were consistent with the measured data and the Voxel interpolation; exceptions included over-predicted Cl and Äspö Brine.

- Voxel analyst interpolation showed general agreement with the measured data, although Meteoric Water was slightly under-predicted and Baltic Sea Water and Cl were over-predicted.

5.2.3 Conclusions

Part of the SKB hydrogeochemical modelling input to Task 5 produced a data set of calculated groundwater mixing proportions for each of the selected control points generated by the M3 approach. Comparison of the measured values with those calculated/predicted by M3 and interpolated by the Voxel program showed a reasonably good correlation, at least considered reasonable enough to be used to calibrate and test the different hydrodynamic models used in Task 5, a central aim of the task.

Svensson et al. (2002) summarised and compared the predicted vs measured data in several figures, two of which are reproduced below (*Figs. 5-6, 5-7*).

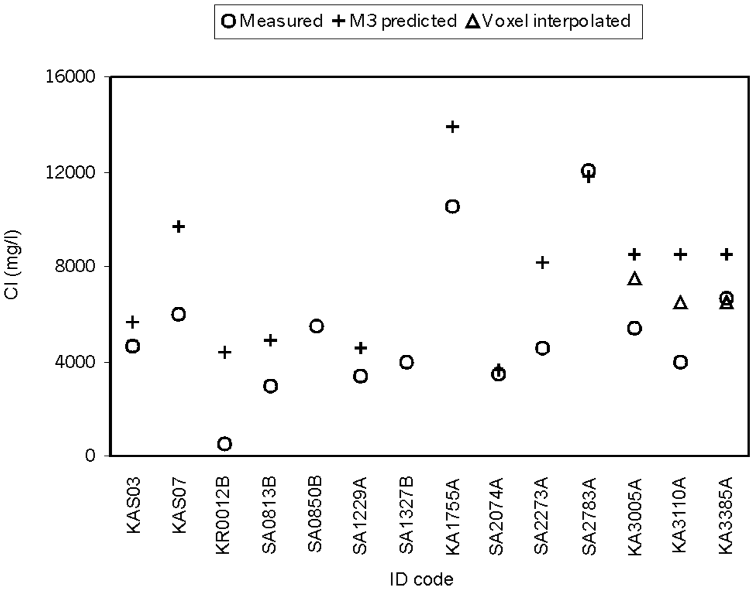


Figure 5-6. *Comparison of the predicted values using M3 and Voxel interpolation with measured data (given values) of Cl (mgL) for the control points. No predictions were made for the control points SA0850B and SA1327B because of a lack of time-series measurements.*

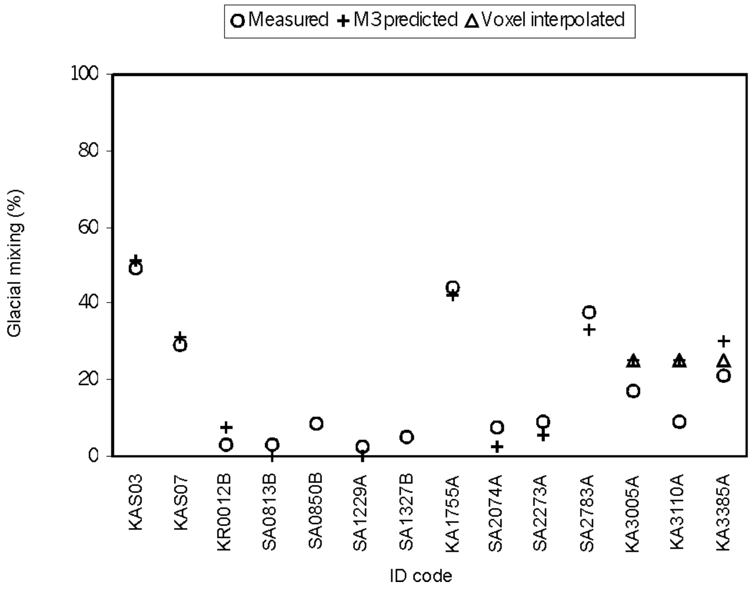


Figure 5-7. *Comparison of the predicted values using M3 and Voxel interpolation with measured data (given values) of Glacial mixing proportion (%) for the control points. No predictions are made for the control points SA0850B and SA1327B because of a lack of time-series measurements.*

5.3 Summary of data usage for the hydrodynamic and hydrogeochemical modelling

The available data for the modelling were sent out in batches (see Appendix 1). The main technical reference for the distributed data was *Rhén et al (1997a)* but some additional written comments to the data accompanied the data sets.

The modelling teams were asked to judge how useful the distributed data had been (see Appendix 1 and *Figs. 5-8 to 5-10*). The judgements were grouped into six classes:

P = data of great importance for quantitative estimation of model parameters
p = data of less importance for quantitative estimation of model parameters
M = data of great importance used qualitatively for setting up model
m = data of less importance used qualitatively for setting up model
X = data useful as general background information
- = data not used

Note that these judgements should not be seen as an illustration of how **exactly** the data were used, but rather a rough view of the usefulness of different data sets. In addition, some data sets indicated “data not used” but it is obvious that at least some of the data have been used.

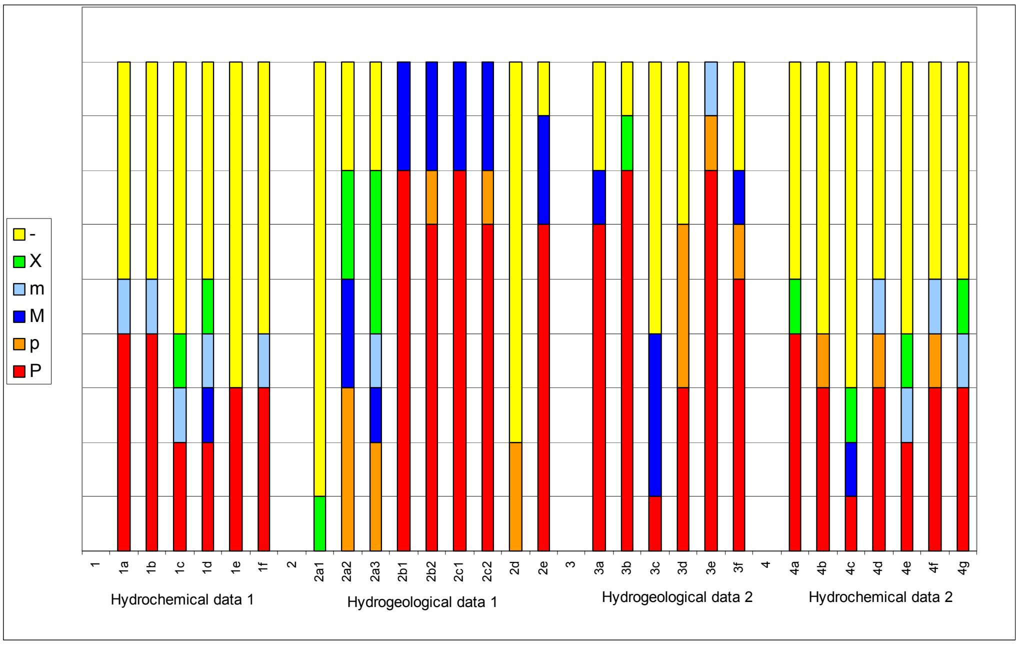


Figure 5-8. *Data usage. The vertical axis indicates the number of each class of data usage (P, P, M, m, X and -); the horizontal axis indicates the different data sets distributed to the modellers (see Appendix 1 and text in section 5.3). The total No of classes for each data set is 9, i.e. equivalent to the No of modelling groups.* ***P*** *= data of great importance for quantitative estimation of model parameters;* ***p*** *= data of less importance for quantitative estimation of model parameters;* ***M*** *= data of great importance used qualitatively for setting up model;* ***m*** *= data of less importance used qualitatively for setting up model;* ***X*** *= data useful as general background information,* ***-*** *= data not used.*

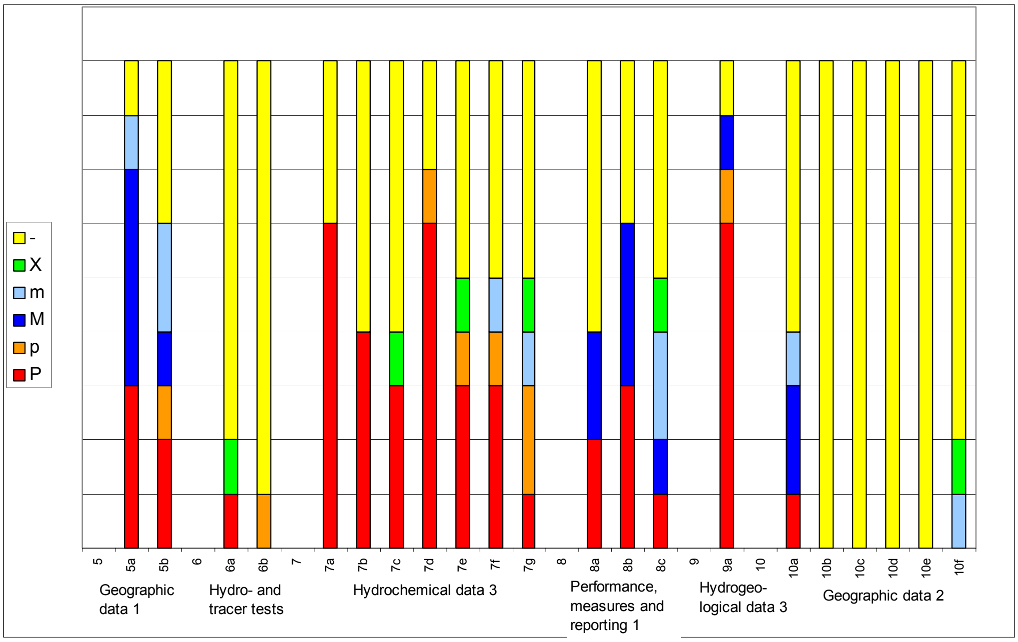


Figure 5-9. *Data usage. The vertical axis indicates the number of each class of data usage (P, P, M, m, X and -); the horizontal axis indicates the different data sets distributed to the modellers (see Appendix 1 and text in section 5.3). The total No of classes for each data set is 9, i.e. equivalent to the No of modelling groups.* ***P*** *= data of great importance for quantitative estimation of model parameters,* ***p*** *= data of less importance for quantitative estimation of model parameters;* ***M*** *= data of great importance used qualitatively for setting up model,* ***m*** *= data of less importance used qualitatively for setting up model,* ***X*** *= data useful as general background information,* ***-*** *= data not used.*

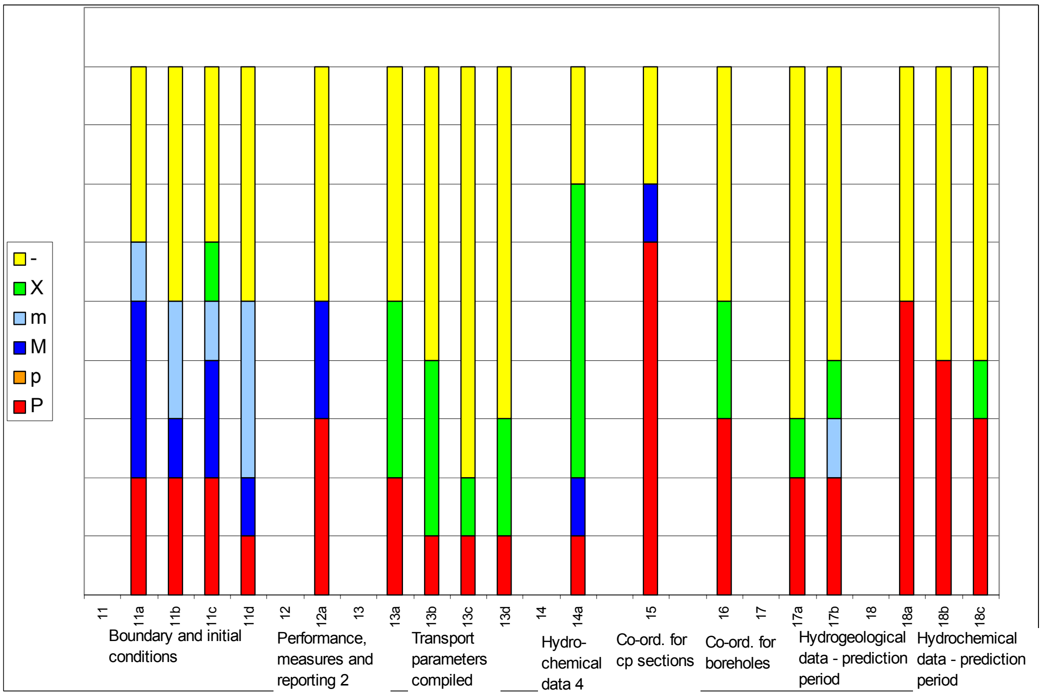


Figure 5-10. *Data usage. The vertical axis indicates the number of each class of data usage (P, P, M, m, X and -); the horizontal axis indicates the different data sets distributed to the modellers (see Appendix 1 and text in section 5.3). The total No of classes for each data set is 9, i.e. equivalent to the No of modelling groups.* ***P*** *= data of great importance for quantitative estimation of model parameters;* ***p*** *= data of less importance for quantitative estimation of model parameters;* ***M*** *= data of great importance used qualitatively for setting up model;* ***m*** *= data of less importance used qualitatively for setting up model;* ***X*** *= data useful as general background information;* ***-*** *= data not used.*

Twenty data sets for the Task 5 modelling were sent out. The first data sets were aimed at defining geometries, boundary and initial conditions as well as data for calibration of the models. Some data were hidden for predictive purposes. It was decided that a number of boreholes in tunnel section 2900 to 3600 m should be control points for the predictions; later two more control points situated in boreholes drilled from surface were added. The tunnel front was at chainage 2900m on February 1st 1994 and at 3600 m on September 16th 1994. Several data sets containing information gathered after February 1st 1994 were sent out after the first predictions had been made. The sequence of different data deliveries is listed below:

1. *Hydrogeochemical Data Set 1* consisted of all raw data sampled at the surface and from the tunnel boreholes, except for the boreholes along tunnel section 2900 to 3600m

2. *Hydrogeological Data Set 1* consisted of:

    - meteorological data (annual mean air temperature, precipitation and evapotranspiration), dates of the tunnel and shaft positions, tunnel and shaft geometry,
    - hydrochemistry of the water measured at the weirs along the tunnel (i.e. chloride, pH, Electrical Conductivity), and
    - geometry of the suggested HCDs.

3. *Hydrogeological Data Set 2* consisted of:
    - monthly mean flow rates measured at the weirs for tunnel section 0-2900m (during the period May 1991–January 1994),
    - piezometric levels (estimated undisturbed levels; daily values from July 1st 1991-24th of January 1994; 30 day mean from June 1st 1991-May 21st 1993),
    - salinity in borehole sections and measurement pipes (to calculate the actual pressure at measurement section based on the piezometric levels), and
    - coordinates for the borehole sections.

Later all available measured flow rates for the entire tunnel were sent out to all modellers before the actual predictions were made (i.e. Data Set 9a).

4. *Hydrogeochemical Data Set 2* presented:
    - mixing proportions (from borehole sections and as grid data based on inter- and extra-polation),
    - boreholes characterised by more comprehensive time series measurements, and
    - borehole sections interpreted to intersect or lie close to the HCDs.

5. *Geographic Data Set 1* consisted of the Äspö coastline, topography of Äspö and the surrounding area.

6. *Hydrotests and Tracer Tests* were delivered as 19 interference tests and one long-term pumping and tracer test (LPT2).

7. *Hydrogeochemical Data Set 3* represented an update of Data Delivery 4 to replace No 4 (i.e. Hydogeochemical Data Set 2).

8. *Performance Measures and Reporting No. 1* constituted Data Set 8.

9. *Hydrogeological Data Set 3* comprised the monthly mean flow rates measured at weirs for tunnel section 0-3600m (period May 1991–December 1996).

10. *Geographic Data Set 2* consisted of topographic data for an area larger than supplied in Data Set 5, comprising coordinates for wetlands, lakes, streams, catchments areas and coordinate transformation from system RAK-38 to the Äspö local north map system.

11. *Boundary and Initial Conditions* were made available in terms of pressure and salinity and were based on a regional model study made by SKB and CFE *(Svensson, 1997a)*

12. *Performance Measures and Reporting No. 2* was a revision of the Performance Measures and Reporting No. 1.

13. *Transport Parameters* compiled from different SKB projects comprised Data Set 13.

14. *Hydrogeochemical Data Set 4* was a description of the main groundwater reactions (listed by SKB) to be considered by the Task 5 modelling groups.

15. *Coordinates for Control Points* were delivered as Data Set 15.

16. *Co-ordinates for boreholes* drilled from the tunnel

17. *Hydrogeological data-prediction period* were delivered after the results from the first prediction had been sent in to SKB. The data set consisted of:

    - hydrochemistry of the waters collected at the weirs (period July 1991–December 1995),
    - piezometric levels (daily values from July 1st 1991- December 1996).

18. *Hydrogeochemical data-prediction period* provided mixing proportions for boreholes along tunnel section 2900-3600m:
    - all boreholes,
    - those boreholes with more comprehensive time series measurements, and those borehole sections interpreted to intersect or lying close to the HCDs
19. Comments on tritium values
20. Coastline, roads, grouting etc.

(Data set 19 and 20 was not included in the inquiry how the data was used. Therefor not in the Figures 5-8 to 5-10))

Logically, according to the modelling teams the most important hydrogeological data consisted of the geometries of tunnels, shafts, boreholes (control points) and HCDs, the measured flow rates into the tunnel, and the piezometric levels. Of lesser importance were the undisturbed piezometric levels, boundary and initial conditions, geographic data and the compiled transport parameters. Of minor importance were the meteorological data, chemistry of the weirs, and salinity in borehole sections and pipes. Of minor importance also were the supplied hydro- and tracer-tests, which was somewhat surprising, but may reflect the limited time and resources for the modelling exercise.

The most important hydrogeochemical data set was No 7, which was not surprising since it introduced a new end member for the mixing calculations. Overall, however, only about half of the groups considered the data of great importance. This probably reflects the way the different groups managed to make use of the data, but indicated also the difficulties in assessing the consistency between the groundwater flow models and the available hydrogeochemical data.

Data for the prediction period was considered to be of "some" importance, probably reflecting that only a few groups made attempts to update the models and perform new simulations.

5.4 Hydrodynamic simulations including mixing ratios

The rationale of distributing the results of the M3 modelling to the Task 5 modelling groups was to compare the outcome of the hydrogeochemical mixing model with the results of the hydrodynamic modelling. In this section the hydraulically simulated results of the groundwater mixing ratios are compared to the M3 calculated values; these results are summarised in charts/tables. In Appendix 6 the predictions of the mixing proportions are shown in detail. Since some groups updated their model after the predictions, the results presented in the figures below may thus differ from those in Appendix 6.

As mentioned earlier in the report, a number of control points were chosen in order to make predictions; these are listed in Table 5-3 and illustrated in *Figure 3-7.*

Table 5-3: Control points selected for the Task 5 modelling exercise.

Calibration Section 0-2900 m	Control point No	BH name	Section	Secup (m)	Seclow (m)	Repr. HCD or HRD	Comments
	1	KR0012B				Redox zone	
	2	SA0813B	1	5,6	19,5	NE-4	
	2	SA0850B	1	1	19,8	NE-4	
	3	SA1229A	1	6	20,5	NE-1	Appr. 70 m South of the core of NE-1
	3	SA1327B	1	6	20,3	NE-1	Appr. 30 m North of the core of NE-1
	3	KA1061A				NE-1	Appr 40 m from tunnel centre in direction 11am in the HCD
	4	SA2074A	1	6	38,7	NNW-4	
	5	SA2783A	1	5,8	19,9	NNW-2	Interpreted postion of HCD NNW-2
Optional	6	KA1755A		88	160	EW-1	Southern bransch of EW-1
Prediction Section 2900-3600 m							
	7	KA3005A	app 36	58		HRD	
	8	KA3110A		20,05	28,63	NNW-4	
	9	KA3385A				(NNW-7)	Close to interpreted postion of HCD NNW-7
CP outside tunnel	10	KAS03		609	623		Pre-investigations
	10	KAS03		533	626		Construction phase
	11	KAS07		501	604	NE-1	Construction phase

5.4.1 Summary of hydrodynamic and transport parameters

In this section the calibration results of hydrodynamic and transport parameters are summarised as well as some illustrations of flow paths. This serves as a basis to understand sections 5.4.2 to 5.4.11.

The models were calibrated using undisturbed conditions, particularly concerning pressure and in some cases mixing proportions. The final parameter settings of the models following calibration are shown in *Figures 5-11 to 5-17*. In Appendix 5 the details of the parameter setting are reported.

For some of the HCDs (NE-2, NNW-2, NNW-4, NNW-7) the modelling groups suggested quite different transmissivities, which probably partly reflected the different model realisations (e.g. modelling only HCDs or HCDs and HRDs). Posiva/VTT differed from the other modelling groups in assuming that the transmissivities in the HCDs decrease with depth. Typically the transmissivity decreased about 10 fold at a depth of 500m compared to the surface. Furthermore, the flow porosity for the HCDs decreased with depth in the model but this is not presented since the relevant information could not be extracted from the report.

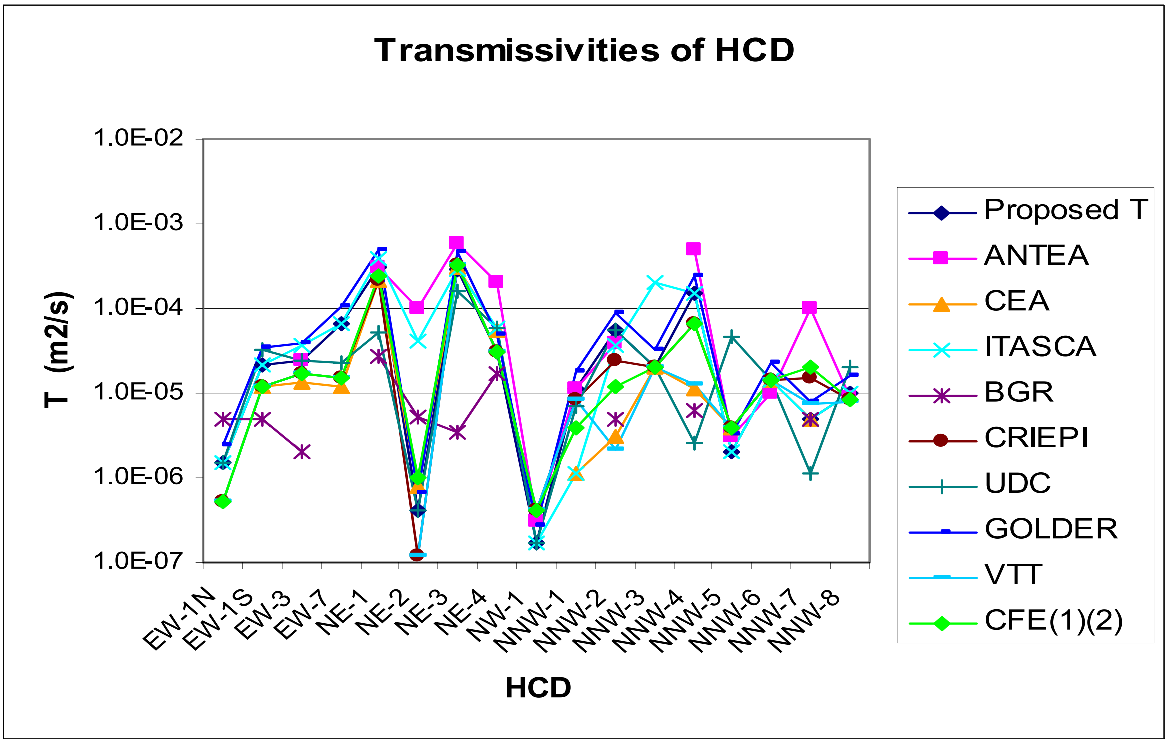
In some cases the transmissivities increased significantly from the suggested values by *Rhén et al (1997a)* probably because of the need to achieve sufficient drawdown (*Figure 5-11*). Considering NE-2, thought to be a low-transmissive feature based on several observations *(Rhén et al, 1997a),* the results suggested that some features were missing or/and that the approach with only HCDs had encountered some difficulties. All modelling groups had problems to model the drawdown when the shafts were excavated, probably due to a large unknown 'feature' near the shafts. Consequently, some modellers indicated that the properties of NE-2 should be modified.

Transient calibration using only the HCDs or a fully 3D simulation might have resulted in larger storativity values for HCDs in a model restricted to only HCDs, compared to a model including both HCDs and HRDs, as illustrated by UDC and BMWi/BGR results.

A rather wide range for the kinematic porosities (or flow aperture) was suggested for the HCDs from the different modelling groups.

The HRDs, the low permeable rock between the HCDs, was modelled by five groups and the results from four of the groups are presented in *Figures 5-15 to 5-17*. The work of Golder was not included since a Discrete Fracture Network (DFN) model was employed which makes it difficult to extract comparable figures. Although the hydraulic conductivity (K) varied significantly between the groups, the presented figures represent constant values in some cases (ANTEA, CRIEPI, VTT) and median values in a stochastic distribution in other cases (CFE, Model 1).

In *Rhén et al. (1997a)* it was suggested that the specific storage (*Ss*) and kinematic porosity (*ne*) could be estimated approximately as a function of K. In *Figures 5-15 to 5-17* these equations have been applied to the median value of K. If a stochastic distribution of K is used for the spatial distribution of the permeability within a HRD, this will influence the mean values of *Ss* and *ne* for the HDRs. In *Svensson (1997b),* a model similar to CFE Model 1, the arithmetic mean of *ne* was calculated to be 0.004 based on the fact that *ne* is never larger than 0.05 in any one cell.



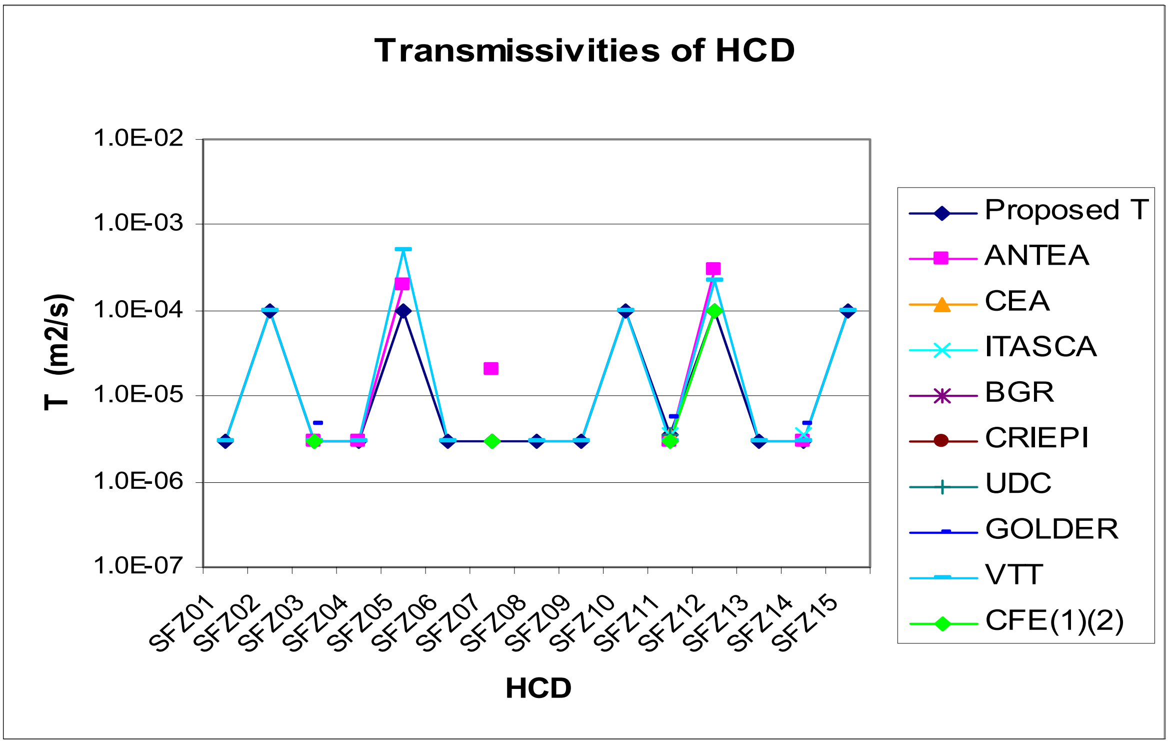
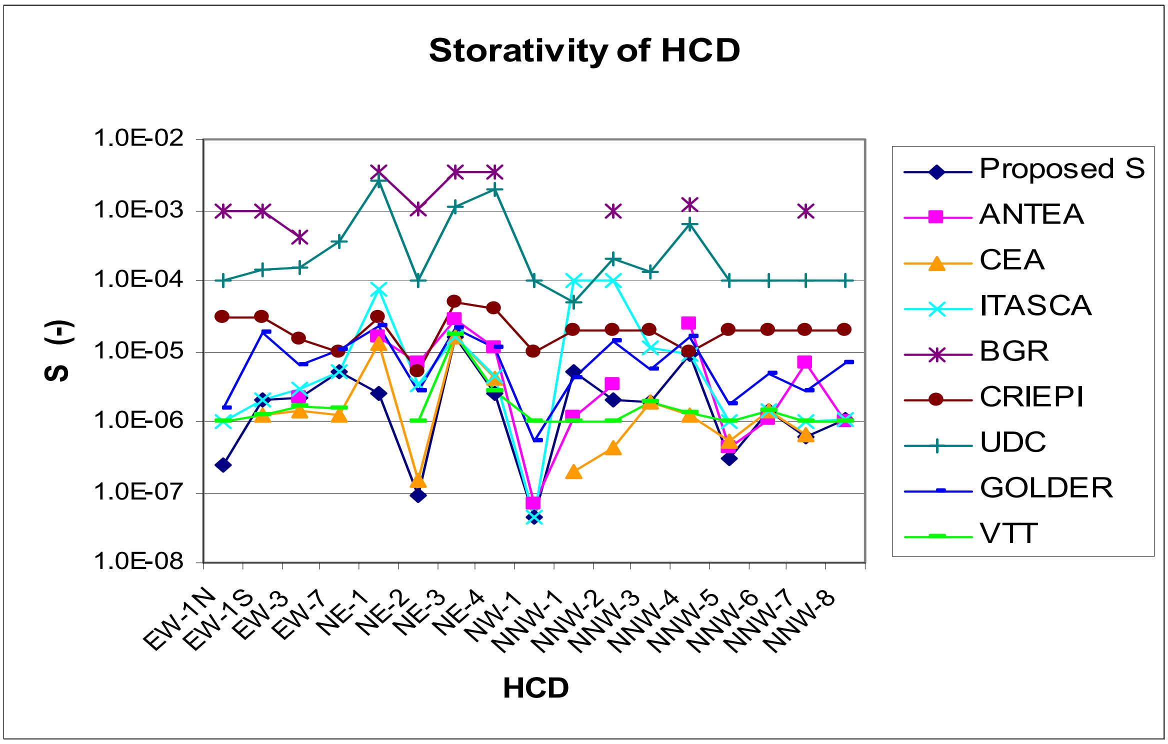


Figure 5-11. *Transmissivity values for the HCDs as proposed (according to Rhén et al., 1997a) and according to the final calibration. In the case of Posiva/VTT the transmissivity in the figure represents the highest value achieved close to surface and also the transmissivity decreases by depth.*



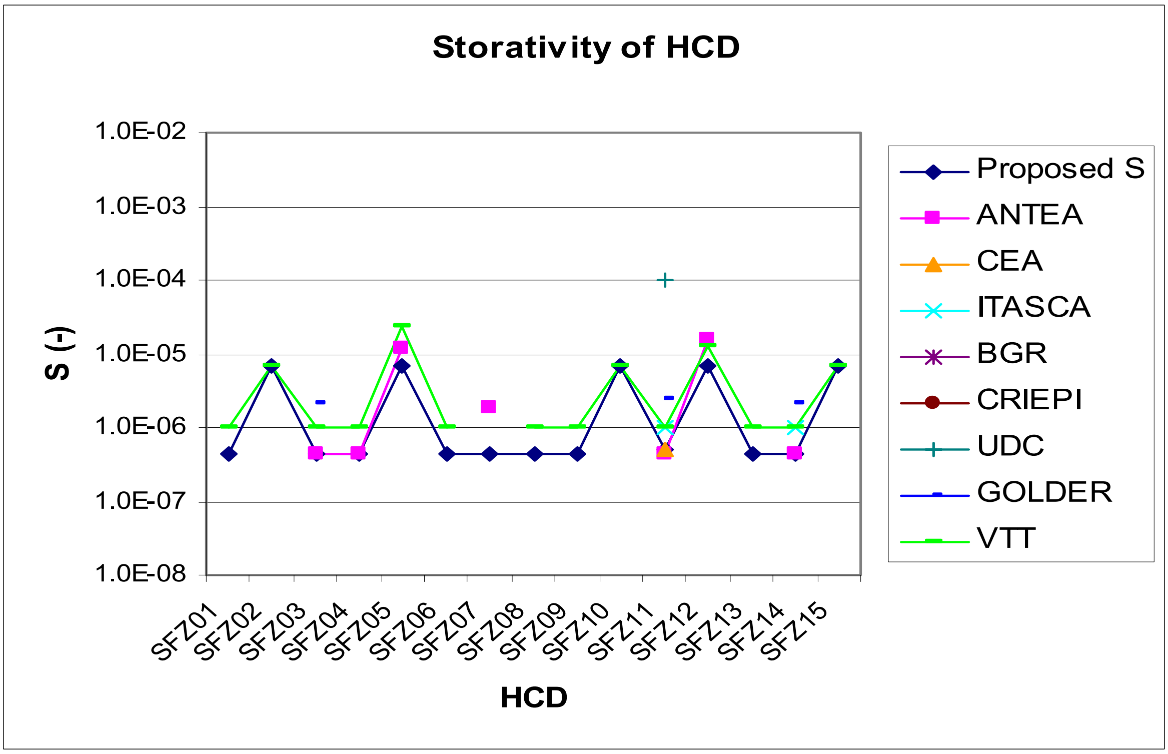
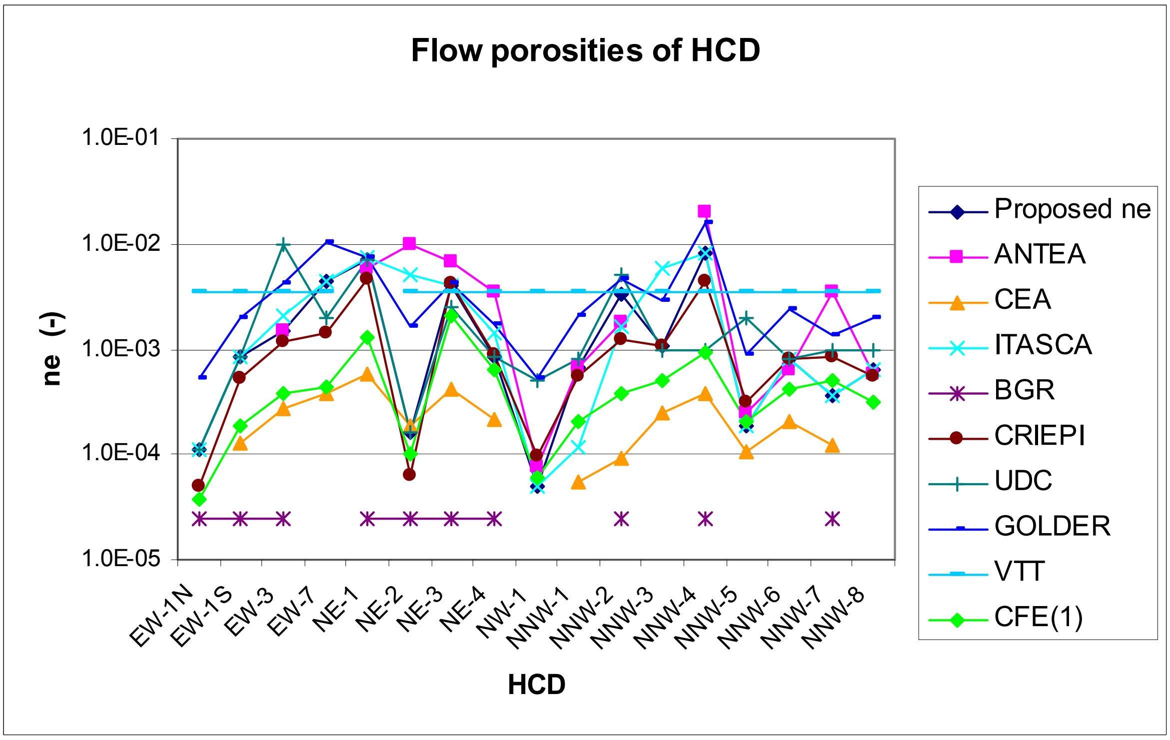


Figure 5-12. *Storativity values for the HCDs as proposed (according to Rhén et al., 1997a) and according to the final calibration. In the case of Posiva/VTT the storativity in the figure represents the highest value achieved close to surface and also the storativity decreases with depth to a minimum value of 1e-6.*



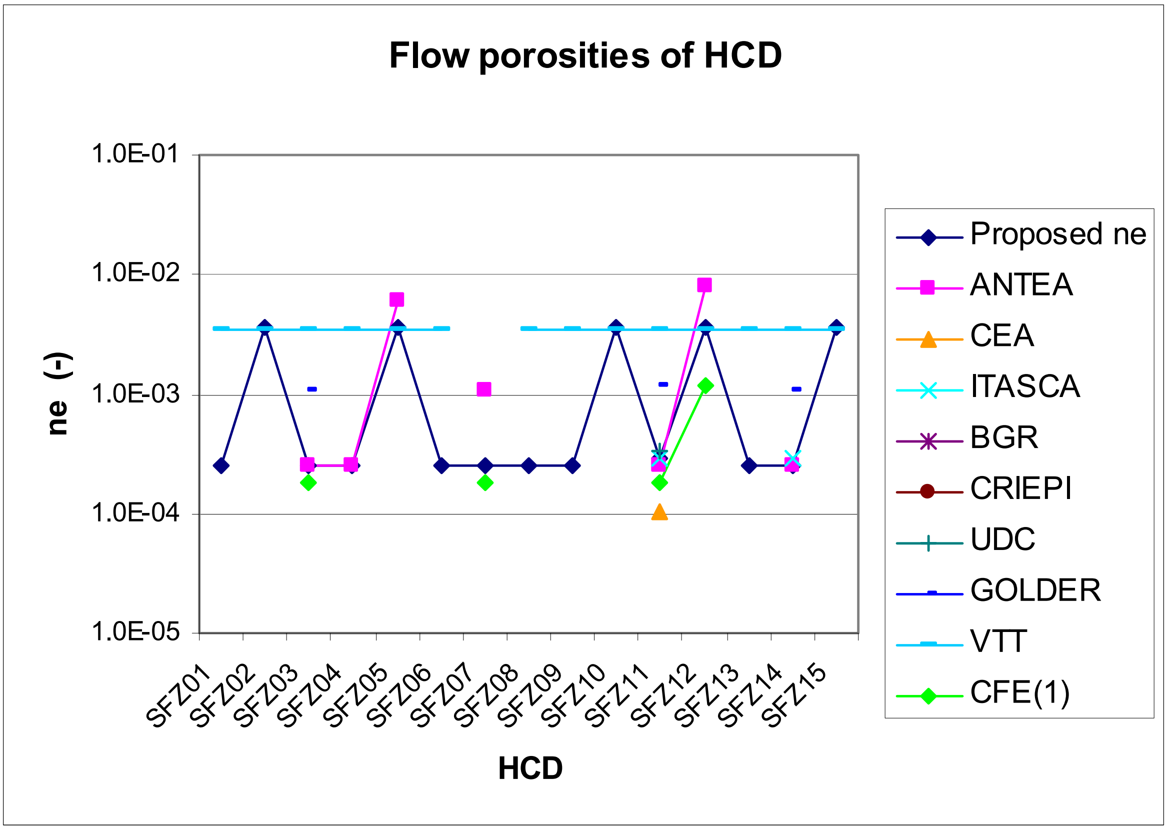
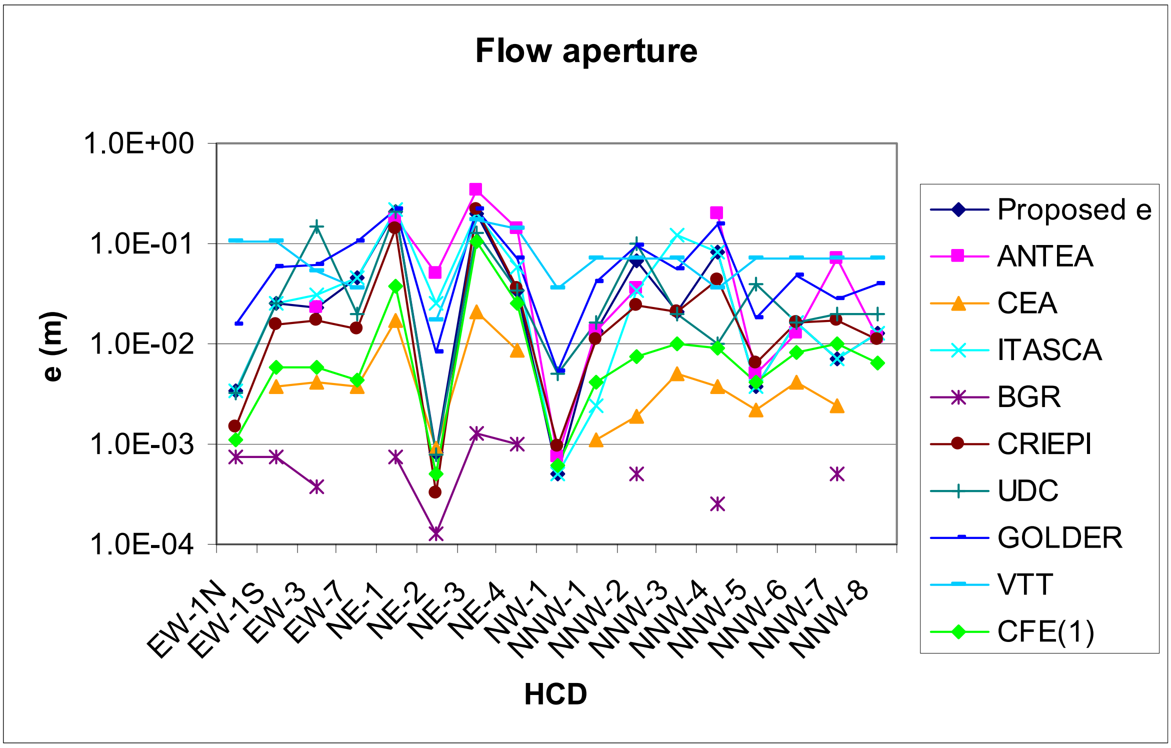


Figure 5-13. *Kinematic porosity values for the HCDs as proposed (according to Rhén et al., 1997a) and according to the final calibration. Corresponding flow aperture is shown in Figure 5-14.*



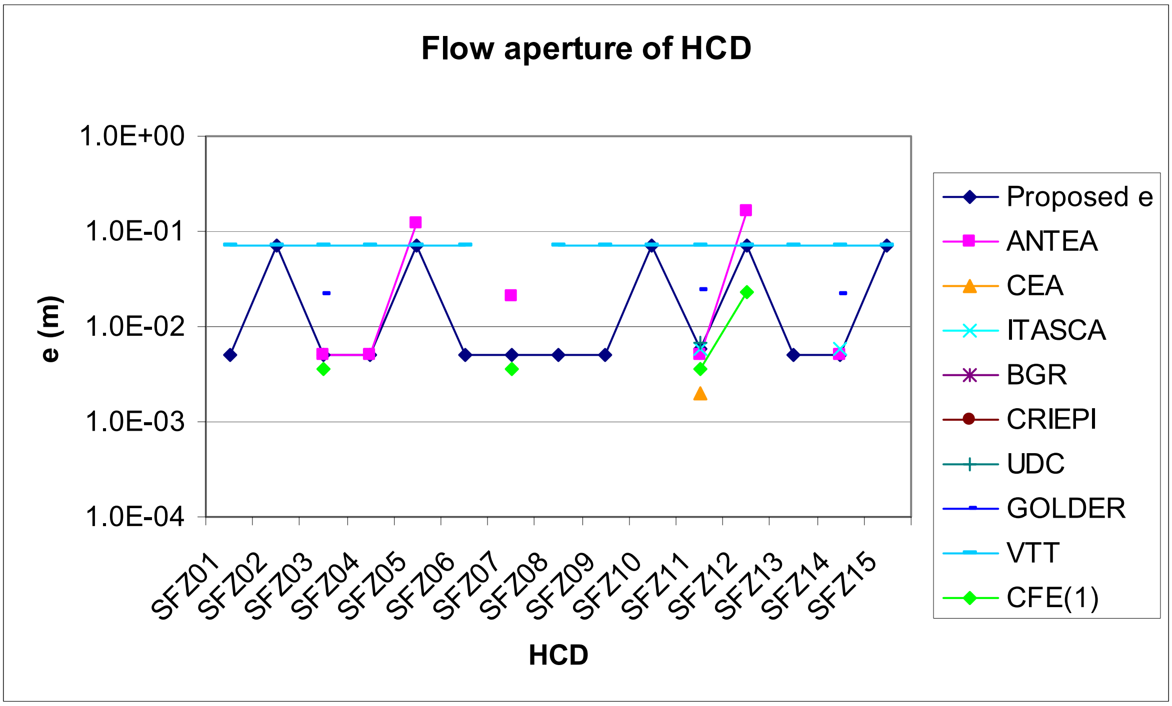


Figure 5-14. *Flow aperture values for the HCDs as proposed (according to Rhén et al., 1997a) and according to the final calibration. Corresponding kinematic porosity is indicated in Figure 5-13.*

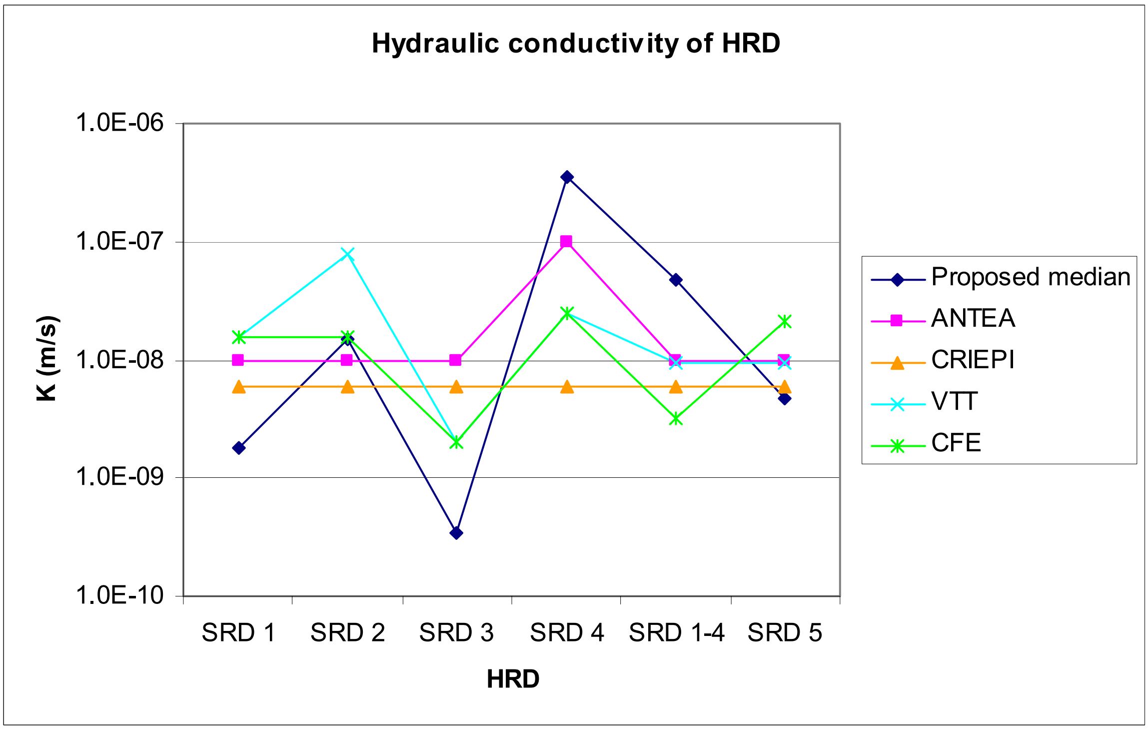


Figure 5-15. *Hydraulic conductivity values for the HRDs proposed (median values coupled to scale from 3m to 300m (see Appendix 5; Rhén et al., 1997a)) and according to the final calibration.*

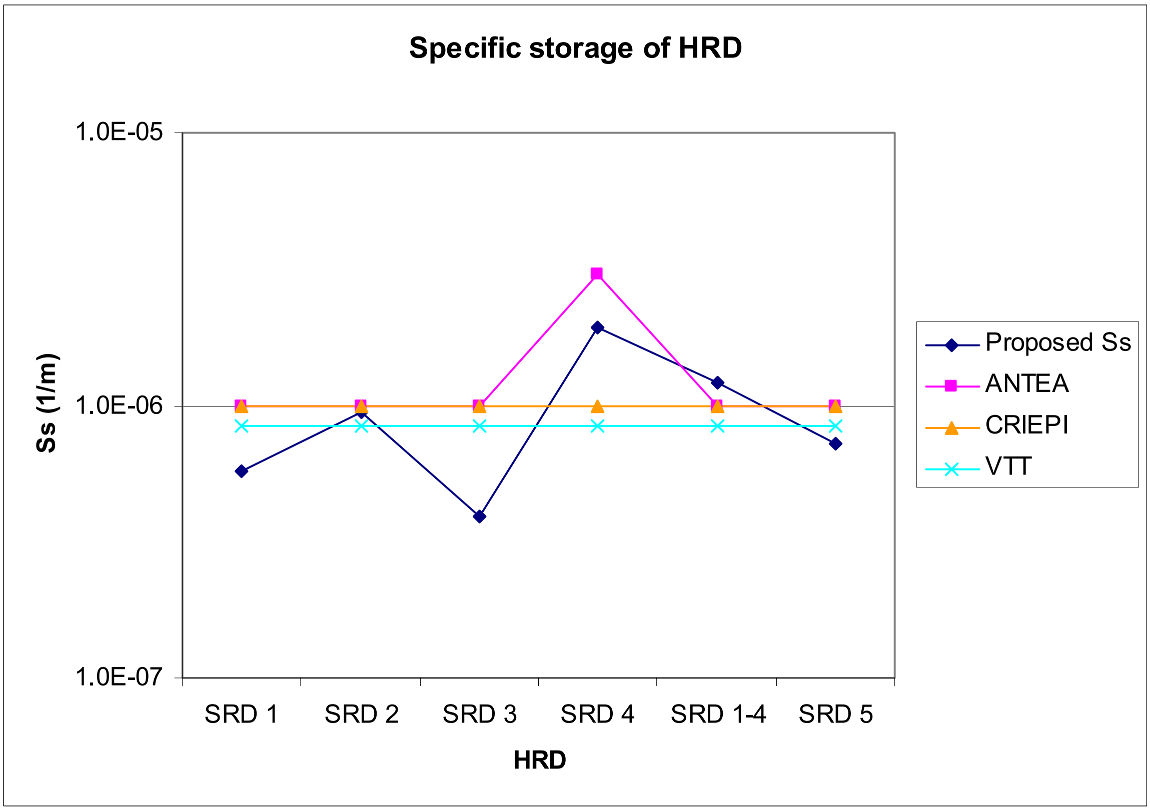


Figure 5-16*. Specific storage values for the HRDs as proposed (after Rhén et al., 1997a) and according to the final calibration.*

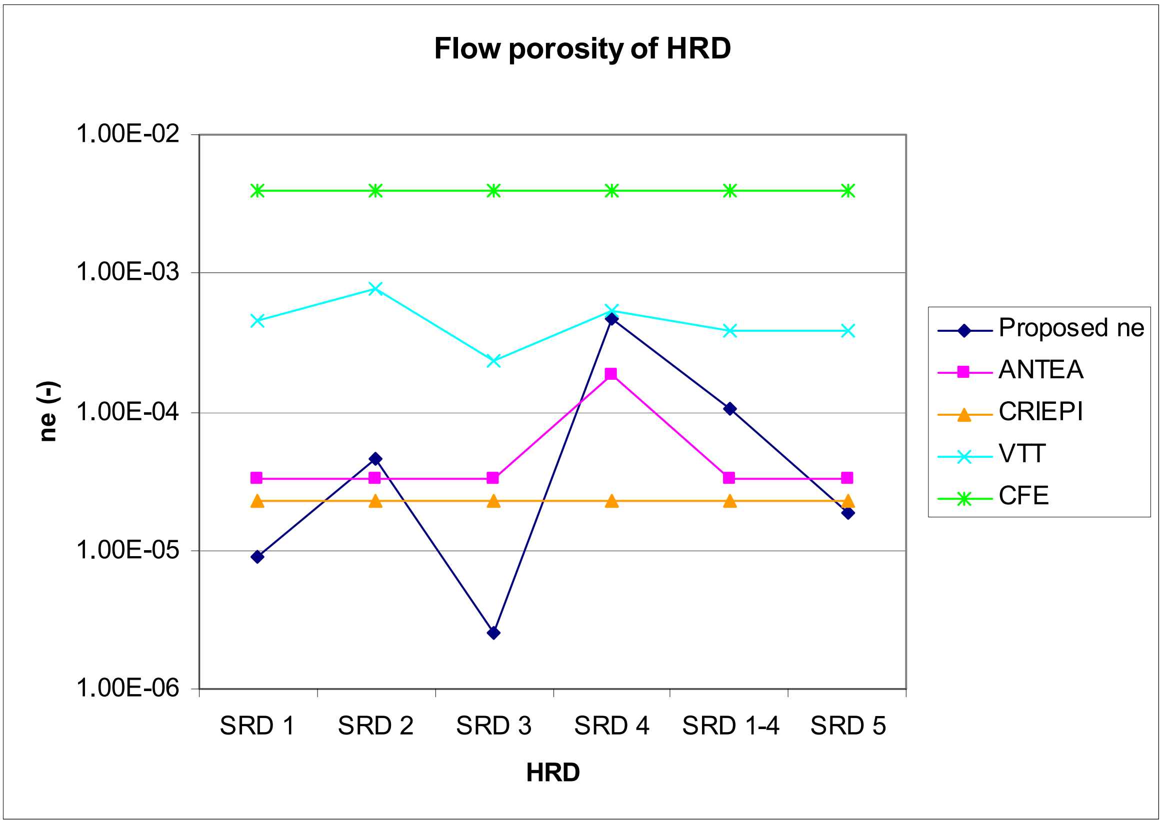
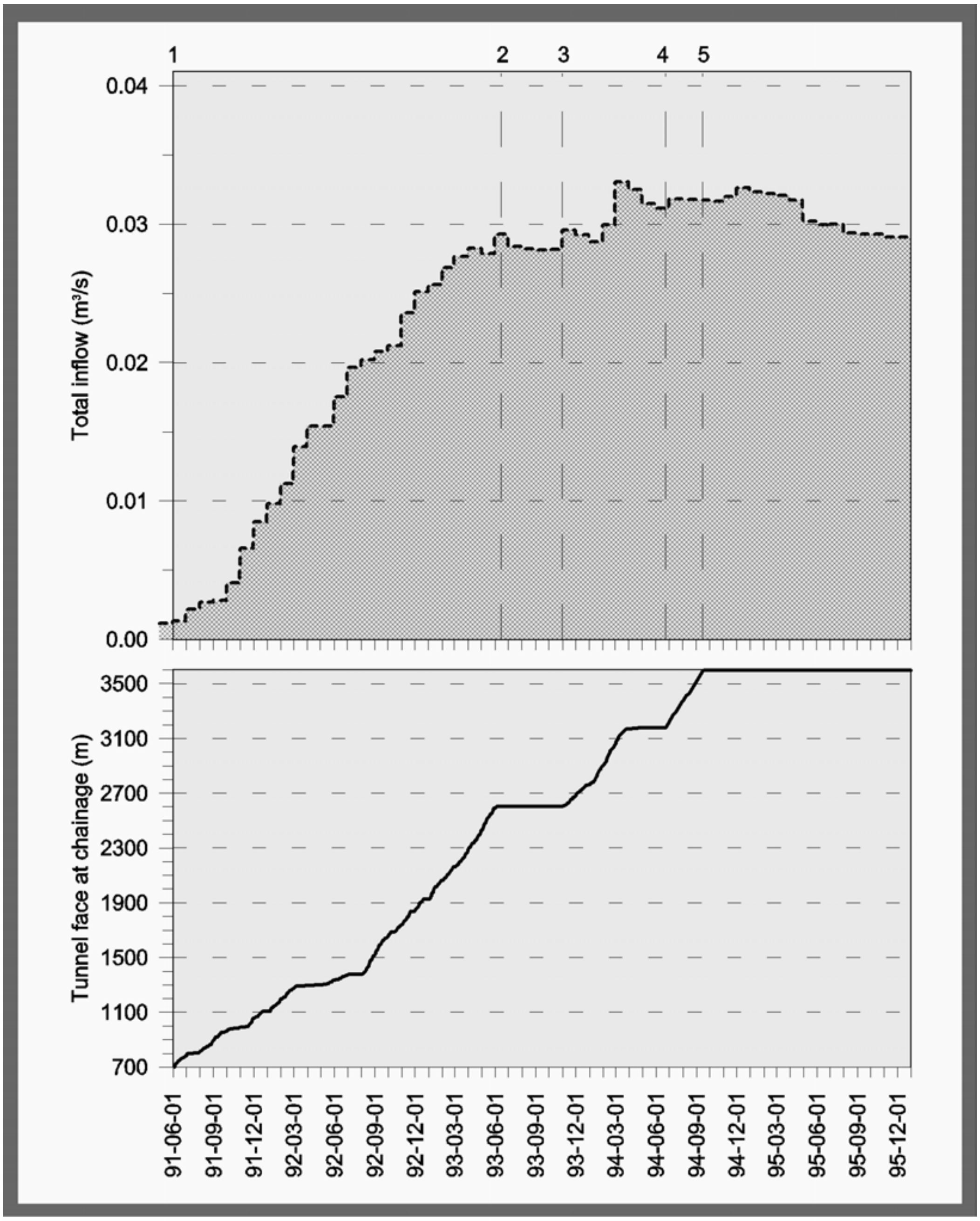


Figure 5-17. *Kinematic porosity values for the HRDs as proposed (after Rhén et al., 1997a) and according to the final calibration.*

In *Figure 5-18* the excavation of the tunnel and the accumulated flow into the entire tunnel is shown. In *Figure 5-19* the flow distribution along the tunnel following tunnel excavation is shown. These data was used as flux boundary condition or as a calibration target with pressure or boundary condition for the tunnel.



1 Passage of tunnelsection 700 m
2 Stop of excavation at 2600 m
3 Start of excavation at 2600 m
4 Start of TBM drilling
5 End of TBM drilling

Figure 5-18. *Flow into tunnel section 0-3600m. The monthly inflow to the tunnel is the sum of the estimated monthly mean inflows measured at each weir along the tunnel (Rhén et al., 1997a).*

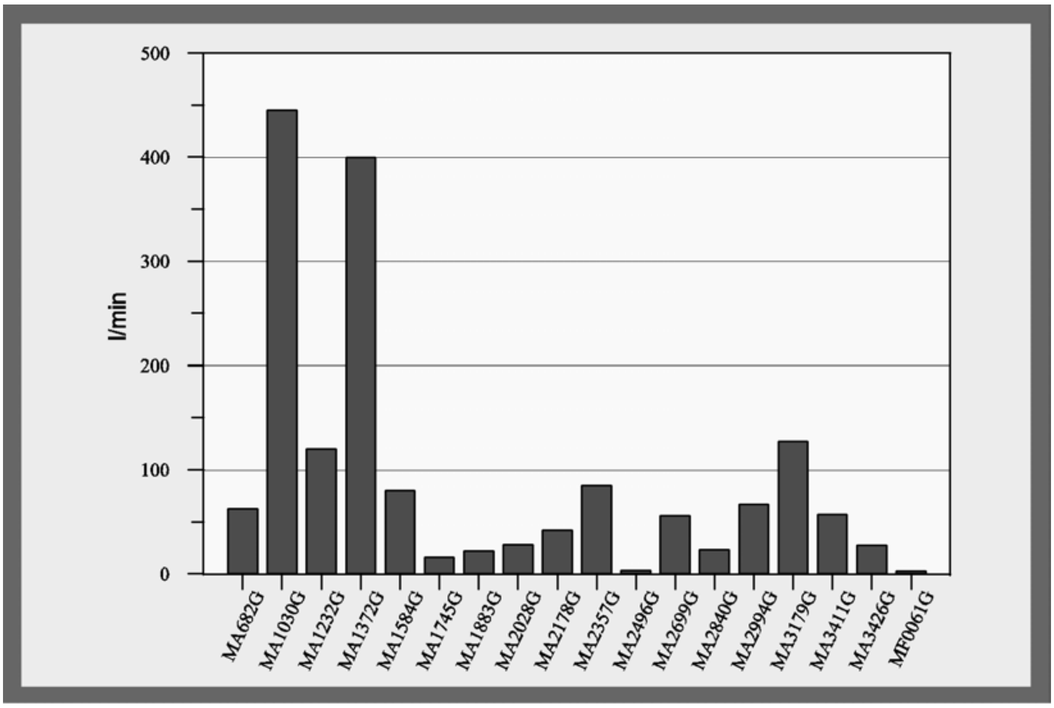


Figure 5-19. *Flow into tunnel sections (monthly mean inflow in October 1995) along the entire tunnel 0-3600m. (* ***MAXXXXG:*** *Measurement point in the tunnel section* ***XXXX****).*

5.4.2 ANDRA/ANTEA

ANDRA/ANTEA constructed a fully 3D model, including HCDs and HRDs, covering the largest volume of rock among the modellers, 3750m x 2620m x 1500 m (*Fig. 5-20*). Constant properties within each HCD and HRD were assumed. On land a constant infiltration was assumed and in sea a constant head. Constant heads and concentrations were applied on the side boundaries. See Table 4-1 for more details about the modelling approach used.

In *Figure 5-21* the water table following tunnel excavation is shown for the calibrated model. The modelled level of the water table compared rather well to the measured levels. No flow paths to the control points along the tunnel were reported.

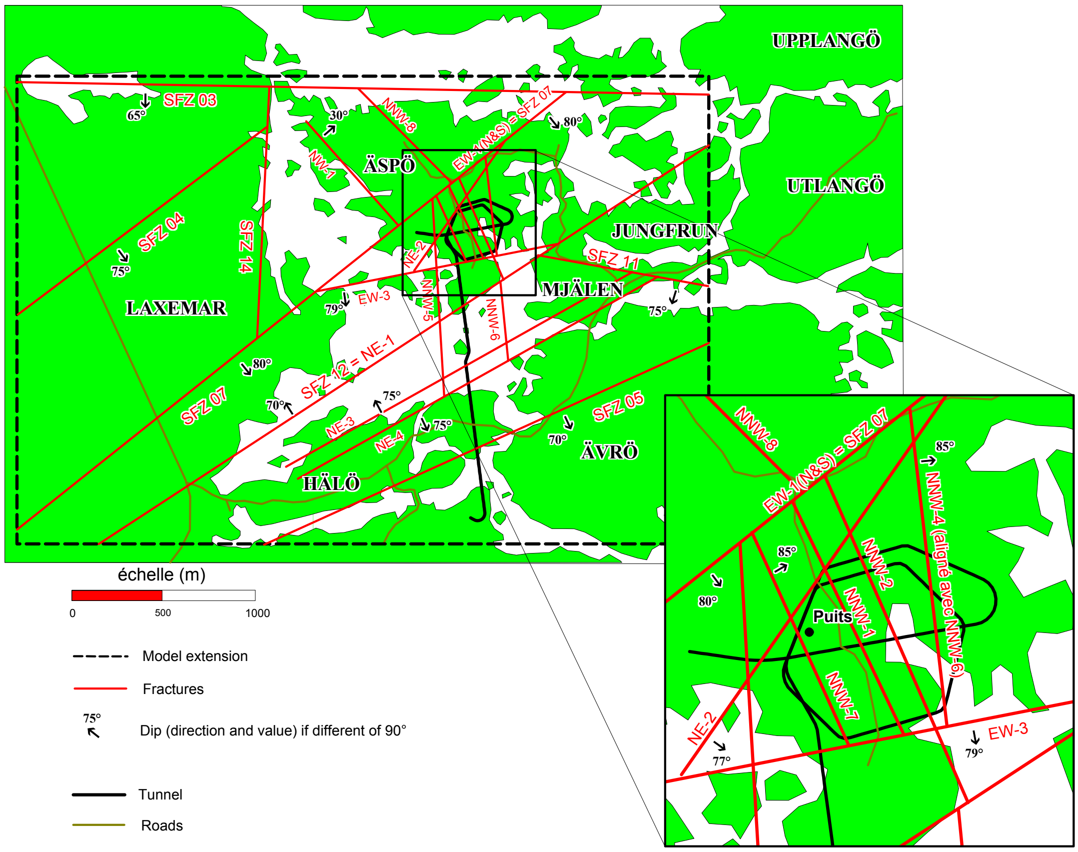


Figure 5-20. Modelled area: ANDRA/ANTEA (Wendling, 2002)

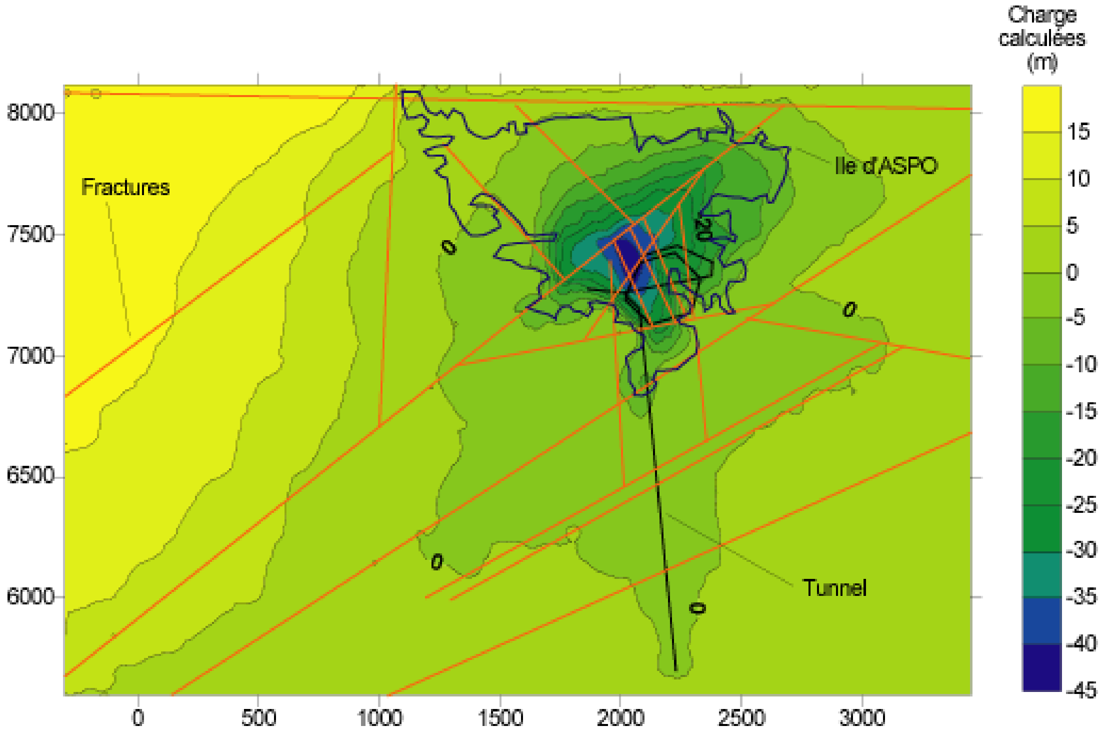
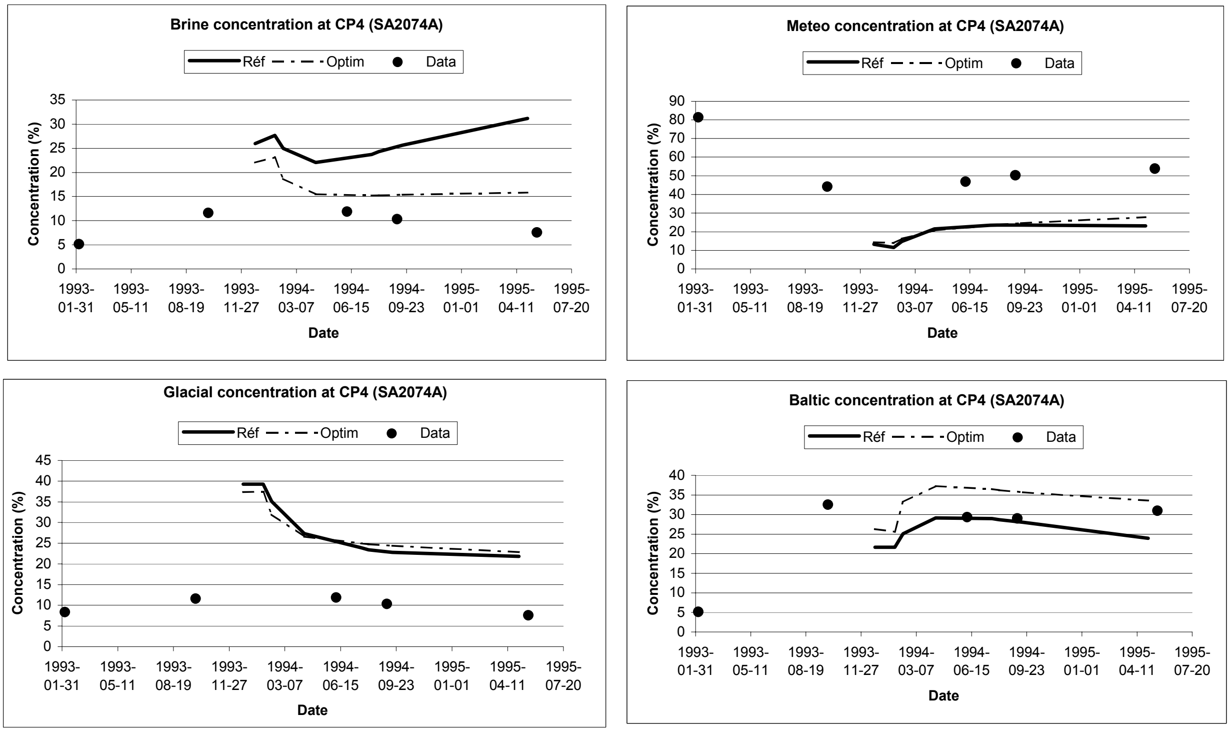


Figure 5-21. The water table for the calibrated model: ANDRA/ANTEA (Wendling, 2002).

ANDRA/ANTEA carried out sensitivity studies to test the suggested transmissivities and hydraulic conductivities, head boundary conditions, kinematic porosities, specific storage and dispersivity based on *Rhén et al. (1997a).* It was concluded that the hydrostatic boundary conditions (instead of taking boundary conditions from the regional model of Svensson (1997)), higher kinematic porosities (by a factor of 10 for some HCDs) and higher specific storage (by a factor of 10 for some HCDs), improved the results. The longitudinal dispersivity of 200m and transversal dispersivity of 20m seemed to result in some improvement. Only minor changes were made for the transmissivities of the HCDs.

What were considered the best results following the sensitivity study are shown in *Figures 5-22* and *5-23*. ANDRA/ANTEA concluded that the improvements for most of the control points were large. It was further concluded that the model corresponded rather well to the measured heads but the modelled concentrations were less satisfactory.



Brine concentration at CP4 (SA2074A)

Meteo concentration at CP4 (SA2074A)

Glacial concentration at CP4 (SA2074A)

Baltic concentration at CP4 (SA2074A)

Figure 5-22. Measured and simulated values of Meteoric, Baltic sea, Glacial, and Äspö Brine waters, at control point 4 (SA2074A) (Wendling, 2002).

Ref. *- Initial parameter distribution based on Rhén et al. (1997a).*
Optim *- Best set of parameters after sensitivity study.*
Data *- Measured values.*

The analysis on general conditions gave important information about mathematical conceptualisation and data treatment:

- The HRDs accounted for 5 to 10% of the calculated concentrations.
- Due to a fine geometric discretisation and a large dispersivity value, time-step duration was not considered a real issue.
- The way initial data were interpolated could modify significantly the results.

- The uncertainty of the M3 concentrations did not cause significant bias in the concentration results (*Summary Report Author's Note: In part this has been questioned by Bath and Jackson, 2002*).

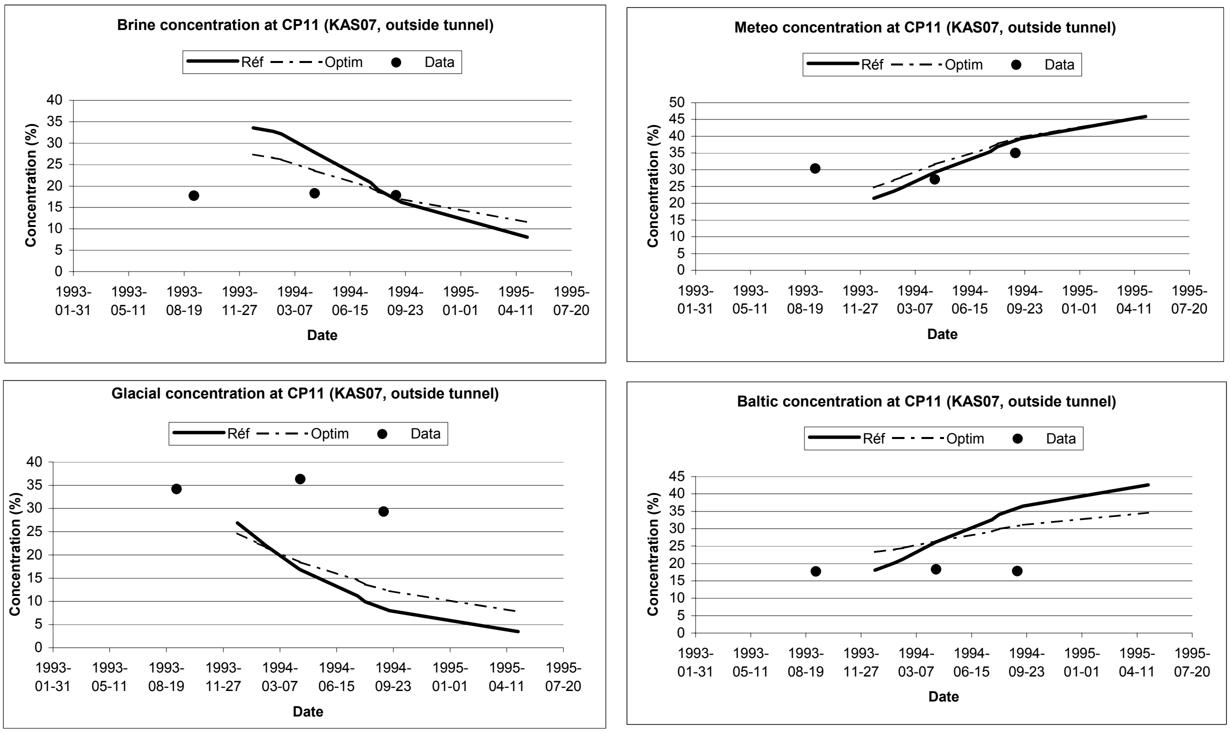


Figure 5-23. Measured and simulated values of Meteoric, Baltic Sea, Glacial, and Äspö Brine waters at control point 11 (KAS07) (Wendling, 2002).

Ref. *- Initial parameter distribution based on Rhén et al. (1997a).*
Optim *- Best set of parameters after sensitivity study.*
Data *- Measured values.*

Analysing the hydraulic and transport parameters the following points were emphasised:

- Calculated concentrations were very sensitive to fracture permeability changes.
- Even though the model was quite large, the boundary head conditions had a very sensitive effect on the results. Although of less importance, this was also true for the concentration boundary conditions.
- Kinematic porosity, specific storage and dispersivity had a sensitive, but less important effect on the calculated concentrations.

The most important features about the Äspö HRL learnt from this exercise were the following:

- The drawdawn created by the tunnel construction had a significant effect on the flow and concentration fields, although much less than the volume generally used to represent the Äspö island in the hydrogeological modelling. Investigating a larger volume to find suitable boundary conditions for the models could be of some interest.

- The influence of the HRDs in the flow and concentration fields (as far as only mixing fractions are concerned) is of second order importance compared to the influence of the fracture network.

5.4.3 ANDRA/CEA

ANDRA/CEA constructed a not fully "3D" model, including the HCDs but not the HRDs, covering an equivalent volume of rock to most of the groups (*Fig. 5-24*). A constant property within each HCD was assumed. See Table 4-1 for more details about the modelling approach used. No flow paths to the control points along the tunnel were reported.

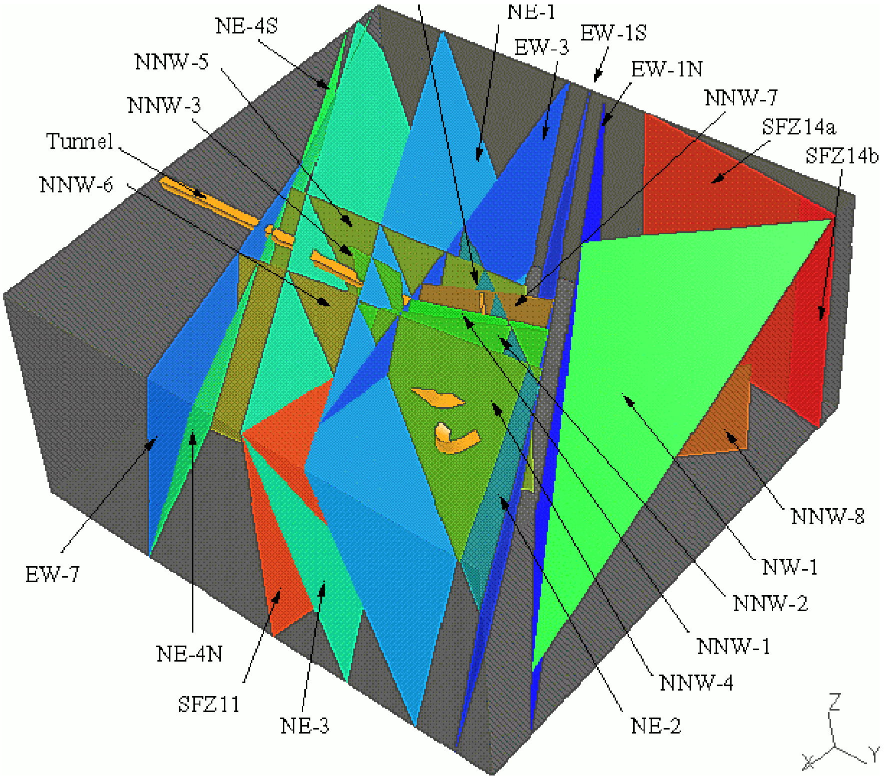


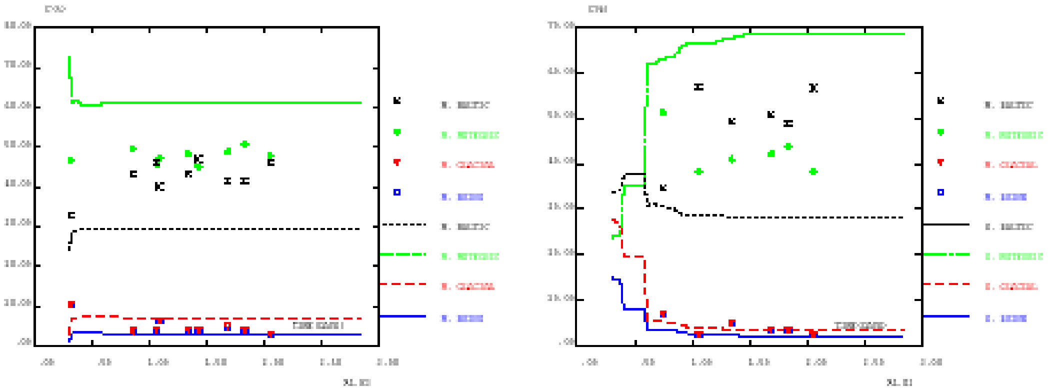
Figure 5-24. *Modelled area: ANDRA/CEA (Grenier and Benet, 2002)*

Figures 5-25 and *5-26* present some results from what was considered to be the best data set. The following conclusions were drawn:

- For the hydraulic problem, a good consistency level was achieved for the model implemented. Nevertheless, the "best solution" provided was not unique as shown by the sensitivity analysis conducted throughout the calibration.

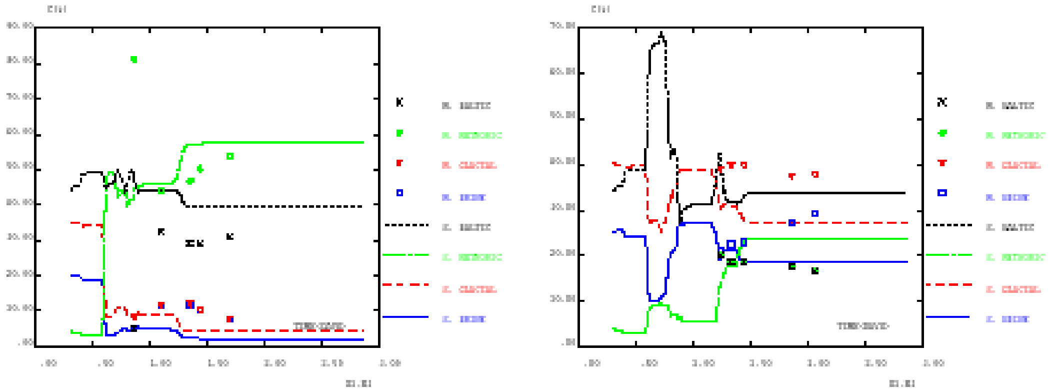
- Incorporation of mixing proportion data into the model allowed for its refinement in the sense that hydraulic calibration of the system required improvement. Nevertheless, preliminary results based on the sensitivity analysis showed that a further level of uncertainty was introduced when transport data was taken into account. This involved uncertainties in transport parameters as well as calibration data such as mixing proportions obtained from M3 based on a few measurements.

- The present level of work on the system did not allow for any conclusions on the global consistency of the model including hydraulic as well as transport data. Nevertheless, uncertainty concerning transport parameters as well as the data were considered important and should be taken into account in the analysis and the calibration strategy.
- From a numerical point of view, future work should lead to the development and implementation of the CASTEM2000 mixed hybrid finite element formulation for flow and transport in a fractured network, where the fractures are considered as being 2D objects. Particle tracking procedures could be adopted also.



(a) Control point 2 (SA0813B-SA0850B)

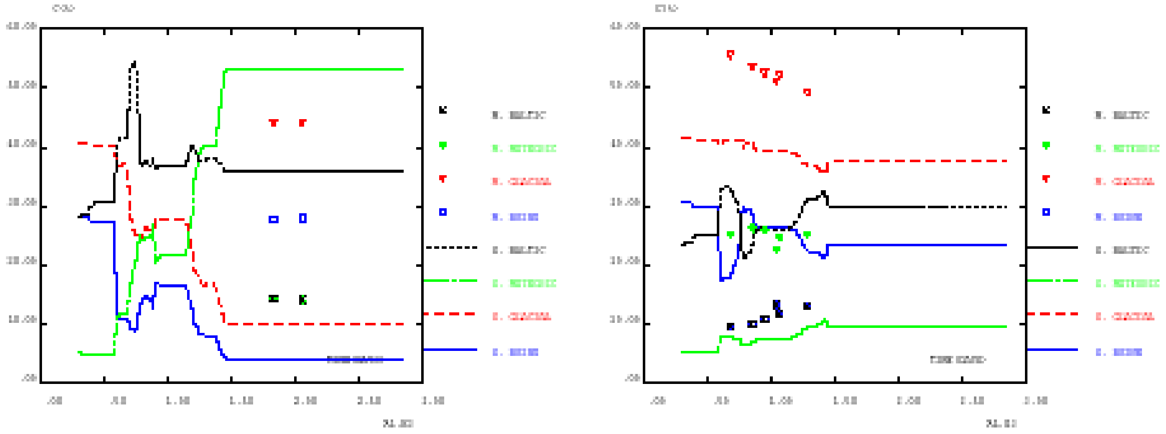
(b) Control point 3 (SA1327B-SA1229A-KA1061A)



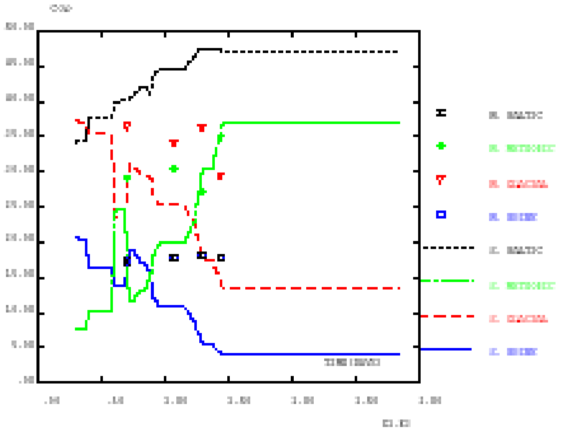
(c) Control point 4 (SA2074A)

(d) Control point 5 (SA2783A)

Figure 5-25. *Measured and simulated values of Meteoric, Baltic Sea, Glacial, and Äspö Brine waters at control points 2, 3, 4 and 5 (Grenier and Benet, 2002).*



(a) Control point 6 (KA1755A) (b) Control point 10 (KAS03)



(c) Control point 11 (KAS07)

Figure 5-26: *Measured and simulated values of Meteoric, Baltic Sea, Glacial, and Äspö Brine waters at control points 6, 10 and 11 (Grenier and Benet, 2002).*

5.4.4 ANDRA/ITASCA

ANDRA/ITASCA constructed a not fully "3D" model, including the HCDs but not the HRDs, covering an equivalent volume of rock to most of the groups (*Figs. 5-27 and 5-28*). Constant properties within each HCD were assumed; the HCDs were modelled according to a pipework model. See Table 4-1 for more details about the modelling approach used.

In *Figure 5-29* the largest flow paths to five control points are shown. Each path was computed up-stream from the control point by branching systematically to the pipe bringing the largest flow rate until a boundary was reached. As expected, the shallowest control points, located under the sea, received mainly water coming from the Baltic Sea, while deeper-sited control points were more influenced by lateral boundaries.

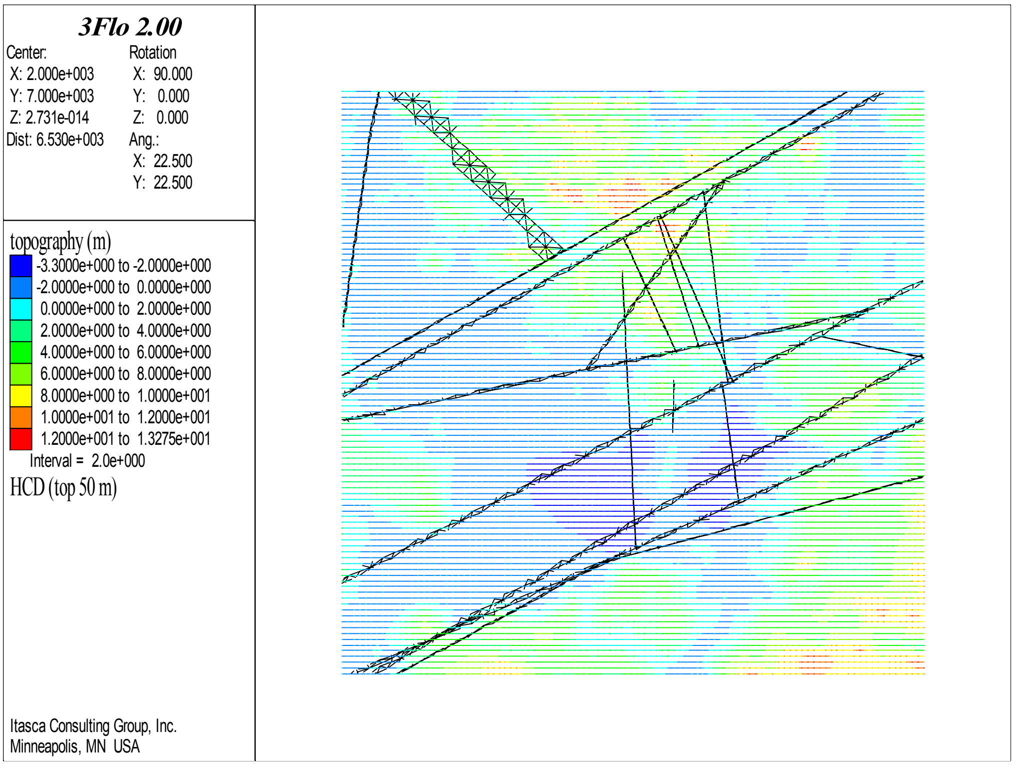


Figure 5-27. *Modelled area: ANDRA/Itasca (Billaux and Paris, 2002).*

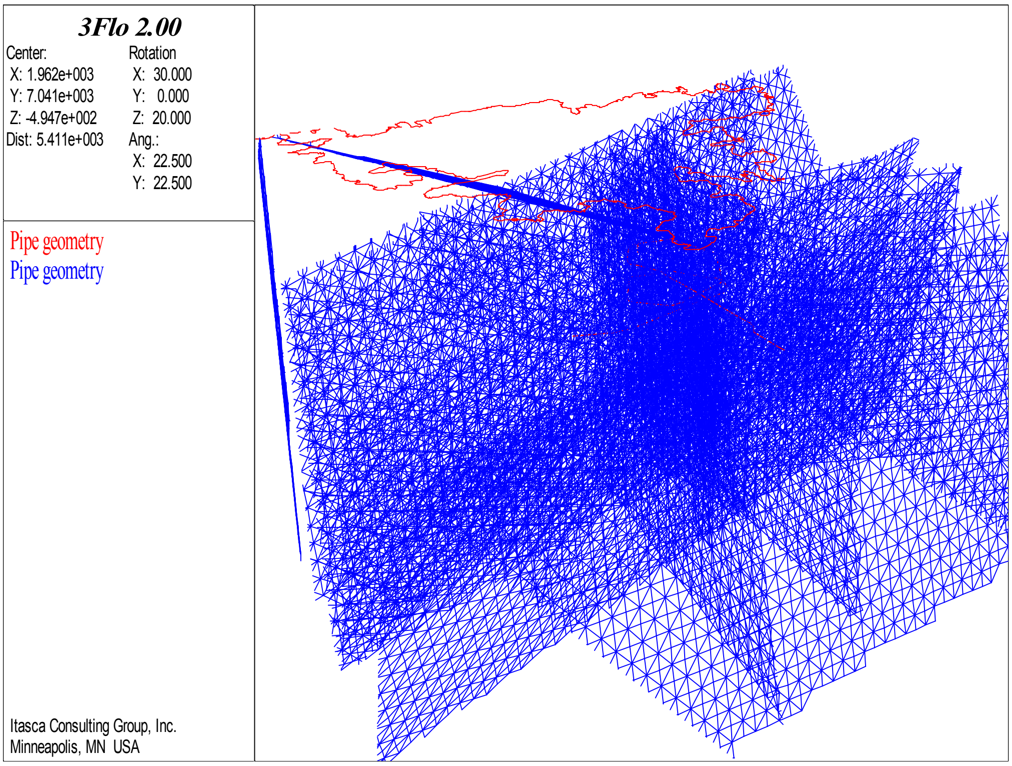
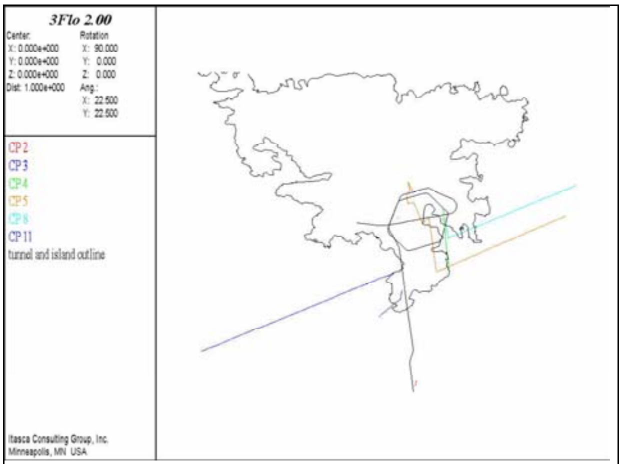
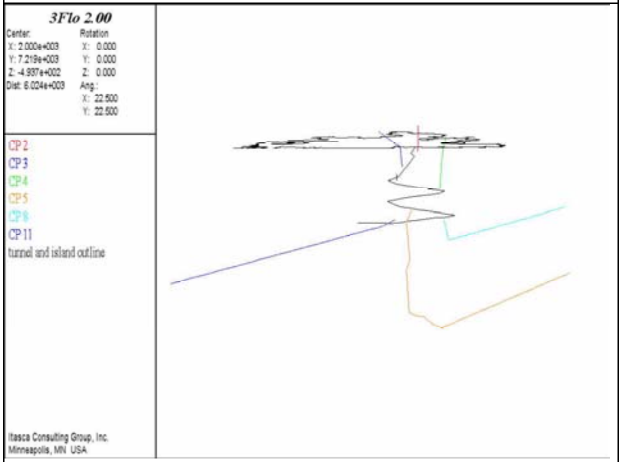


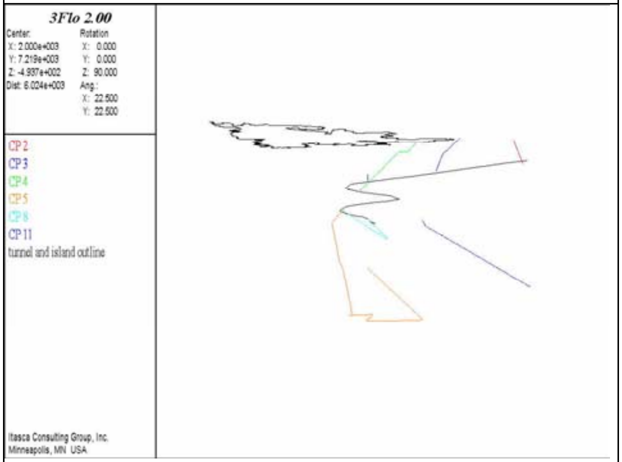
Figure 5-28. *View from SW of the 21 HCDs: ANDRA/Itasca (Billaux and Paris, 2002).*



View from top



View from South



View from East

Figure 5-29. *Flow paths for the largest transport pathways to 5 control points (2, 3, 4, 5 and 11): ANDRA/Itasca (Billaux and Paris, 2002).*

Figures 5-30 and *5-31* show some selected results of the modelled mixing proportions and chlorine concentrations. The conclusions reached were:

- Calibrating the transmissivities of the HCDs to fit piezometric histories in a number of borehole sections proved relatively easy, with only minor changes of the transmissivities needed. It was concluded therefore that the geometrical model was probably rather well established, with the addition of a hydraulic communication between the two EW-1 zones. However, when modelling non-reactive transport and comparing to actual measurements, the "flow-only" calibration proved inadequate; the simulations overestimated the amount of Baltic Water that arrived at the control points.

- New calibrations, which yielded essentially the same quality of fit for heads, but better simulations of chemical end member arrivals, were then performed. The new calibrations were only moderately different, with most of the HCD transmissivities remaining unchanged. This showed that the flow-only fit cannot be unique, since various sets of calibration parameters yielded what looked like acceptable fits. It was emphasised that the use of chemical data, by further constraining the model parameters, helped in obtaining more realistic simulations.

- However, because of the relative scarcity of chemical data, uncertainties remain quite large. Initial chemical compositions were interpolated from a regular grid, itself extrapolated from data points not homogeneously distributed in space. Neither extrapolations nor interpolation took into account the influence of the fractured nature of the medium on the flow. There was no guarantee that the initial conditions derived in this way were at chemical equilibrium.

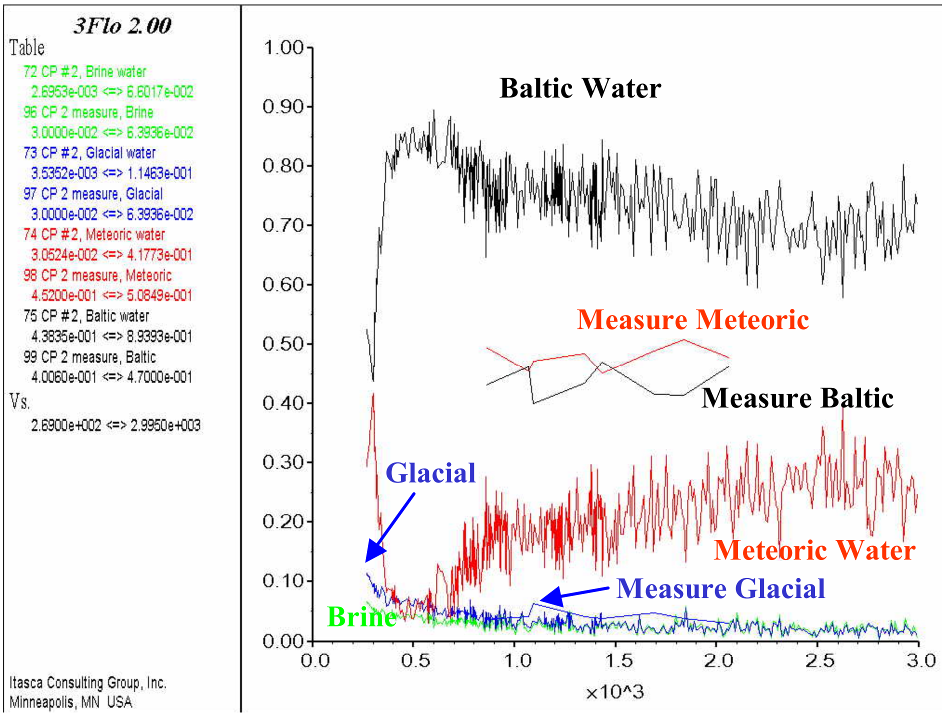
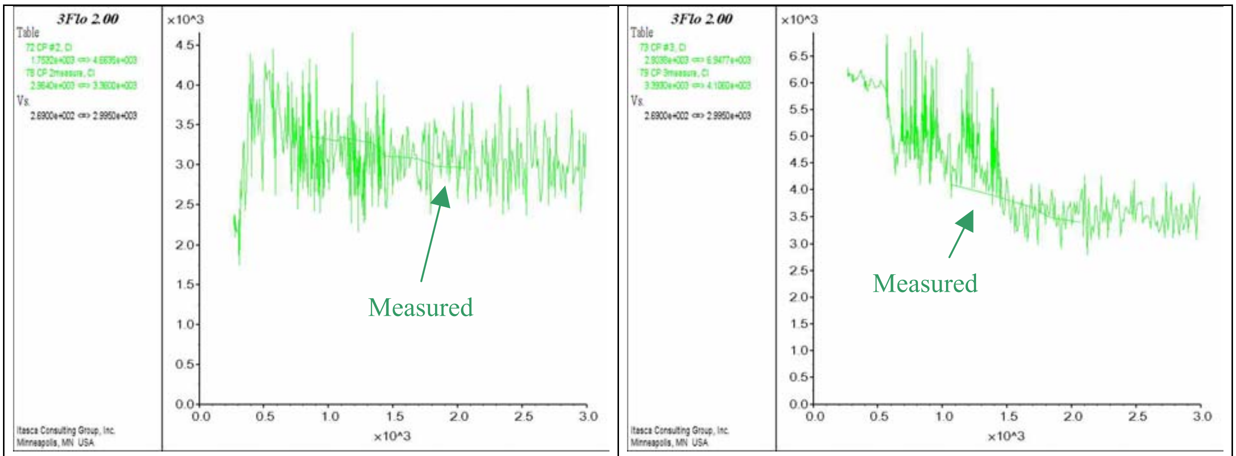
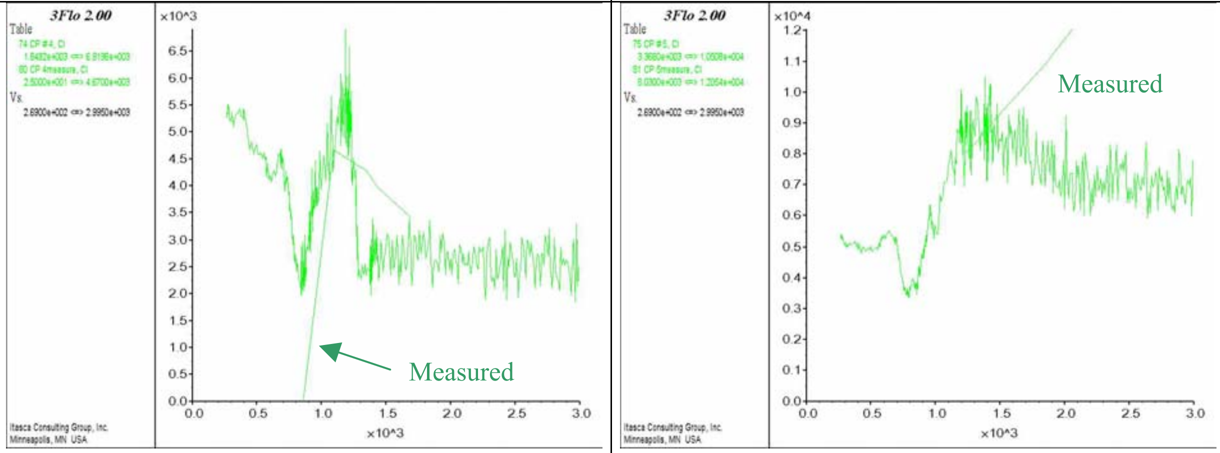


Figure 5-30: *Measured and simulated values of Meteoric, Baltic Sea, Glacial, and Äspö Brine waters at control point 4 (Billaux and Paris, 2002).*



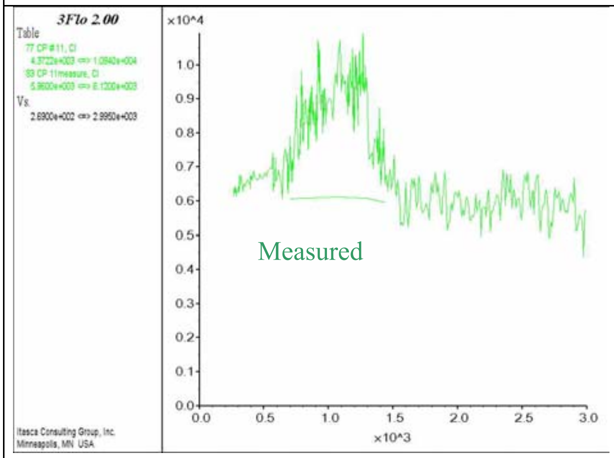
Control Point 2

Control Point 3



Control Point 4

Control Point 5



Control Point 11

Figure 5-31: *Measured and simulated values of salinity in five control points (Billaux and Paris, 2002).*

5.4.5 BMWi/BGR

BMWi/BGR constructed a not fully "3D" model, including the HCDs but not the HRDs, covering an equivalent volume of rock to most of the groups (*Fig. 5-32*). Constant properties within most of the HCDs were assumed. In some HCDs the properties were constant within sub-volumes of the HCDs. See Table 4-1 for more details about the modelling approach used.

In *Figure 5-33* a comparison between measured and simulated head is shown for a few control points.

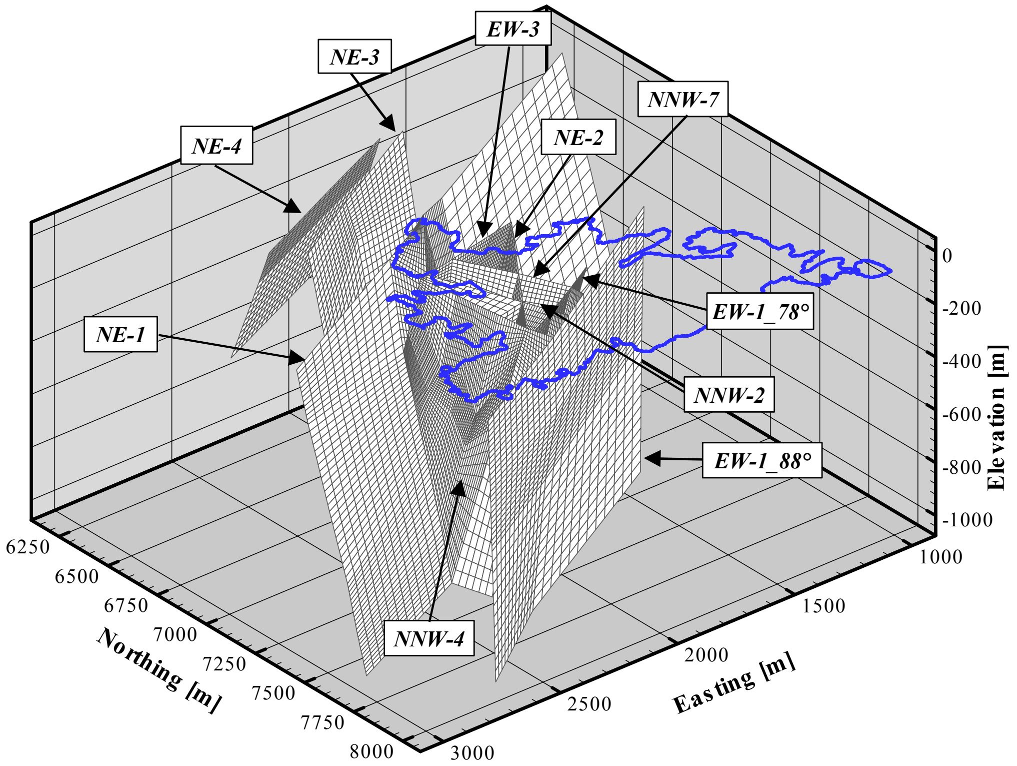


Figure 5-32. *Modelled area: BMWi/BGR (Liedtke and Klennert, 2002).*

Figures 5-34 and *5-35* show selected results of the modelled mixing proportions. The results led to the following conclusions:

- It is important to be aware of the strong influence of the boundary and initial conditions on the modelling results, especially as these conditions were derived from grid data. Adjustment of the sum of the different groundwater types to 100 % may also affect the results.

- There was some difficulty to determine the initial water concentrations in the offshore parts of the model. A sensitivity analysis was considered necessary to test the input and output values of the flow and groundwater mixing models because the results depended mainly on the material properties and boundary conditions.

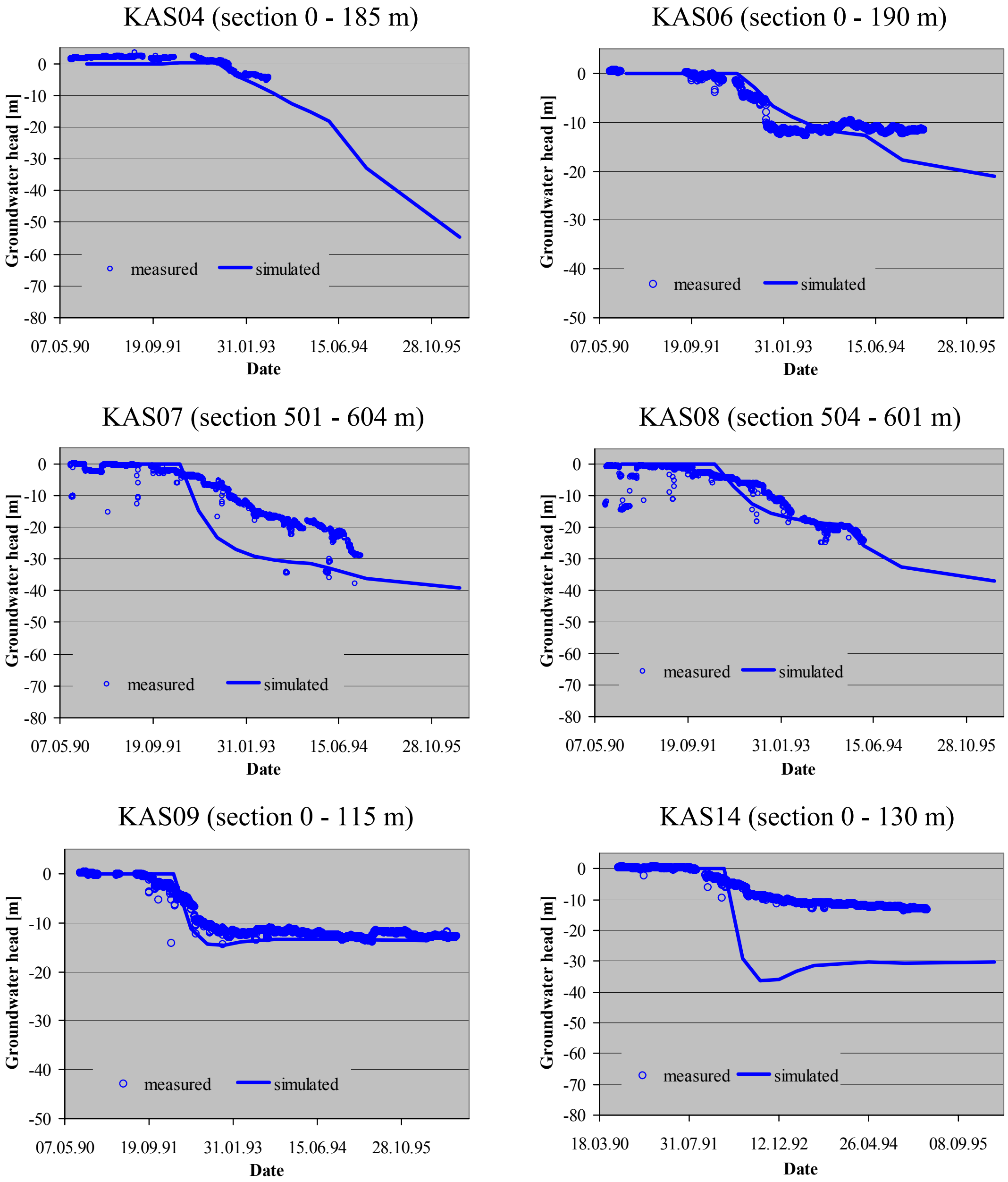


Figure 5-33. *Measured and simulated heads for a few selected control points: BMWi/BGR (Liedtke and Klennert, 2002).*

- Additionally, refinement of the model fracture network and an adjustment to the natural conditions were considered useful in order to account for the spatial variability of the hydraulic and transport parameters as well as the boundary and initial conditions.

- Moreover, it was considered very helpful if both the hydraulic and the chemical results have been available at the control points. The modelling results therefore would have been more accurate and the agreement of the modelled and measured values at the calibration points could have been improved.

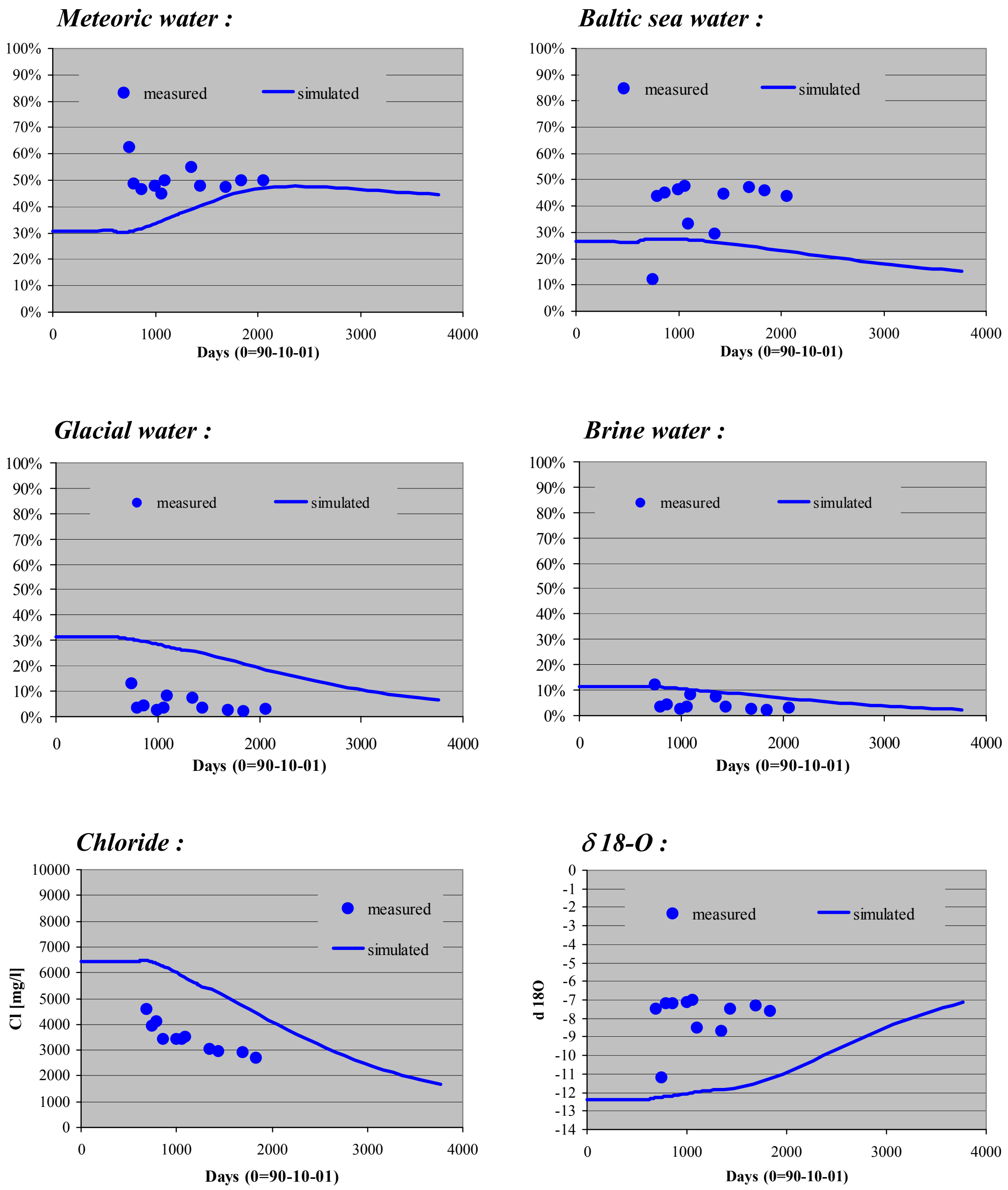


Figure 5-34. *Measured and simulated values of Meteoric, Baltic Sea, Glacial, and Äspö Brine waters, chloride content and* δ^{18}*O at borehole SA1420A (Liedtke and Klennert, 2002).*

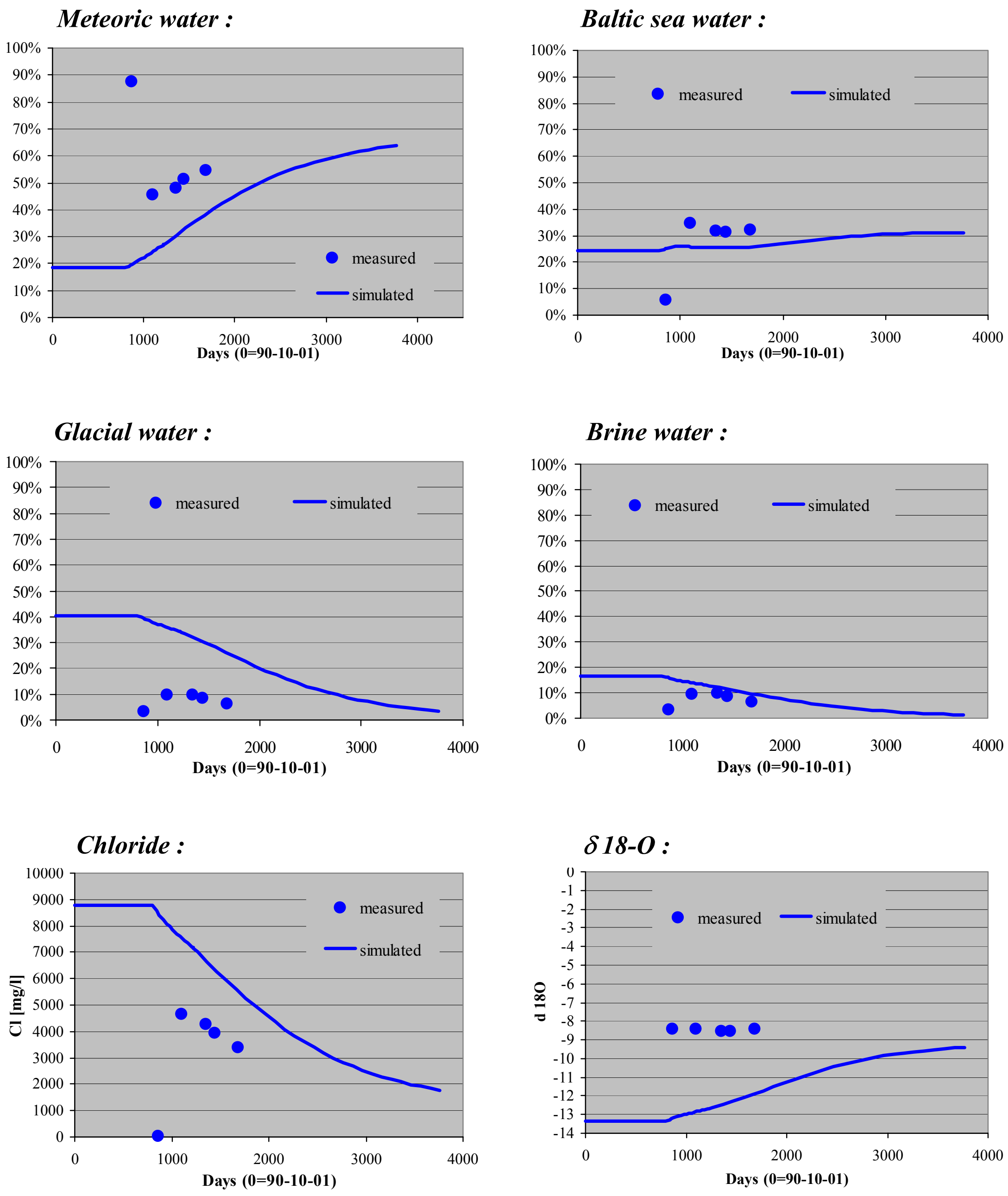
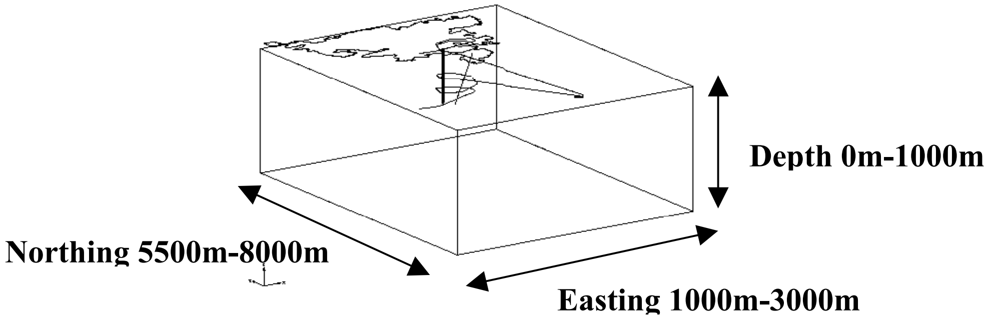


Figure 5-35. *Measured and simulated values of Meteoric, Baltic Sea, Glacial, and Äspö Brine waters, chloride content, and δ^{18}O at borehole SA2074A (Liedtke and Klennert, 2002).*

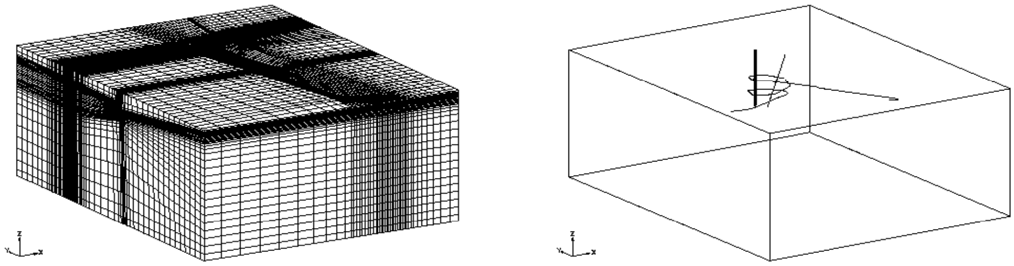
5.4.6 CRIEPI

CRIEPI constructed a fully 3D model, including the HCDs and the HRDs, covering the next largest volume of rock among the modellers (*Fig. 5-36*). Constant properties within each HCD and HRD were assumed. See Table 4-1 for more details about the modelling approach used.

Flow paths to control point 4 (SA 2074) are shown in *Figure 5-37*.



(1) Modeling area



(2) Hexahedral element (3)Line element

***Figure 5-36.** Modelled area: CRIEPI (Hasegawa et al., 2002).*

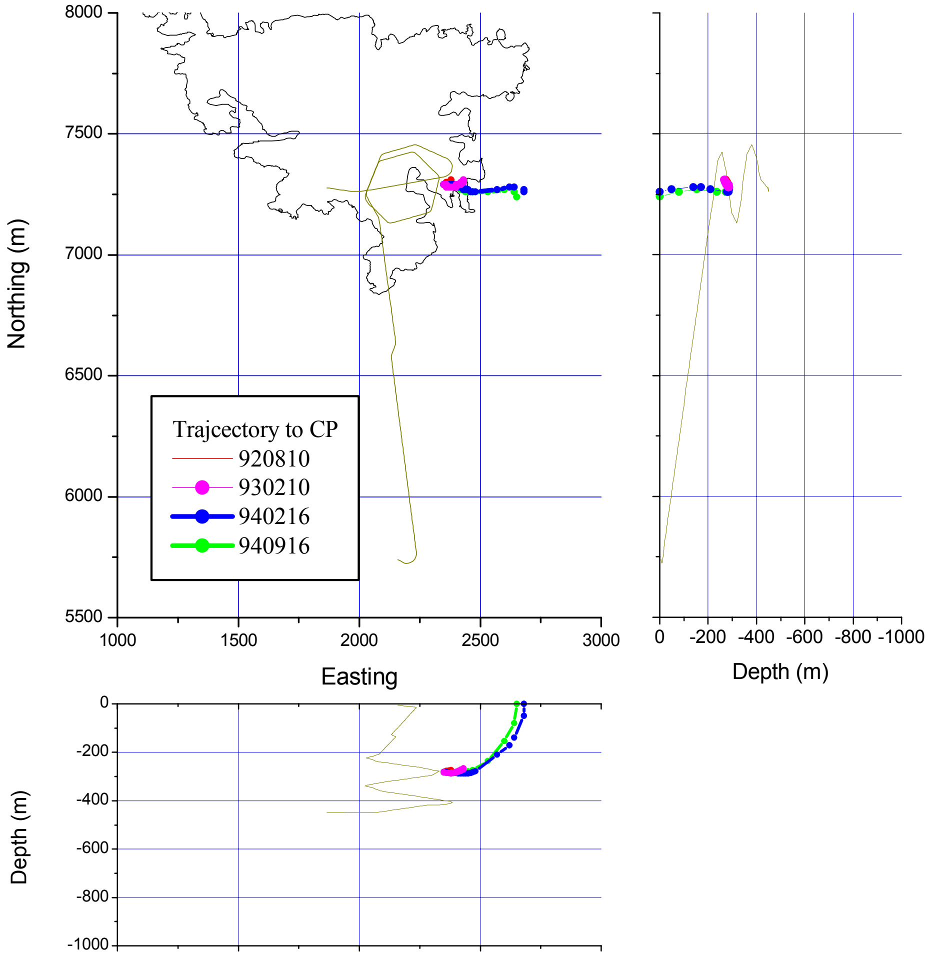


Figure 5-37. Trajectory to monitoring point (SA2074); the colours of lines show the change of trajectory with time: CRIEPI (Hasegawa et al., 2002).

Figures 5-38 and *5-39* show selected results of the modelled mixing proportions and the chlorine and ^{18}O concentrations. The following was concluded:

Groundwater flow

In particular, the hydraulic conductivity of NNW-7 and the HRDs proved to be invaluable in simulating the drawdowns. The HCDs intersecting the spiral tunnel and shaft were important to evaluate drawdowns (e.g. NNW-1, NNW-2, NNW-4, NNW-7, NE-2). It was important to model the HRDs because the hydraulic conductivity, although low, influenced the drawdowns.

The progress of tunnel construction and the time-series of the drawdowns were quite useful to refine the hydrogeological model because these relationships helped to clarify the impact and response. Drawdowns were roughly represented by properly representing the geometric relationship between tunnel, shaft, HCDs and the monitoring borehole sections.

Since the simulated drawdowns represented the timing and amount of drawdown, the hydrogeological model was reasonable from the viewpoint of the geometric and hydraulic properties.

Hydrogeochemical distribution

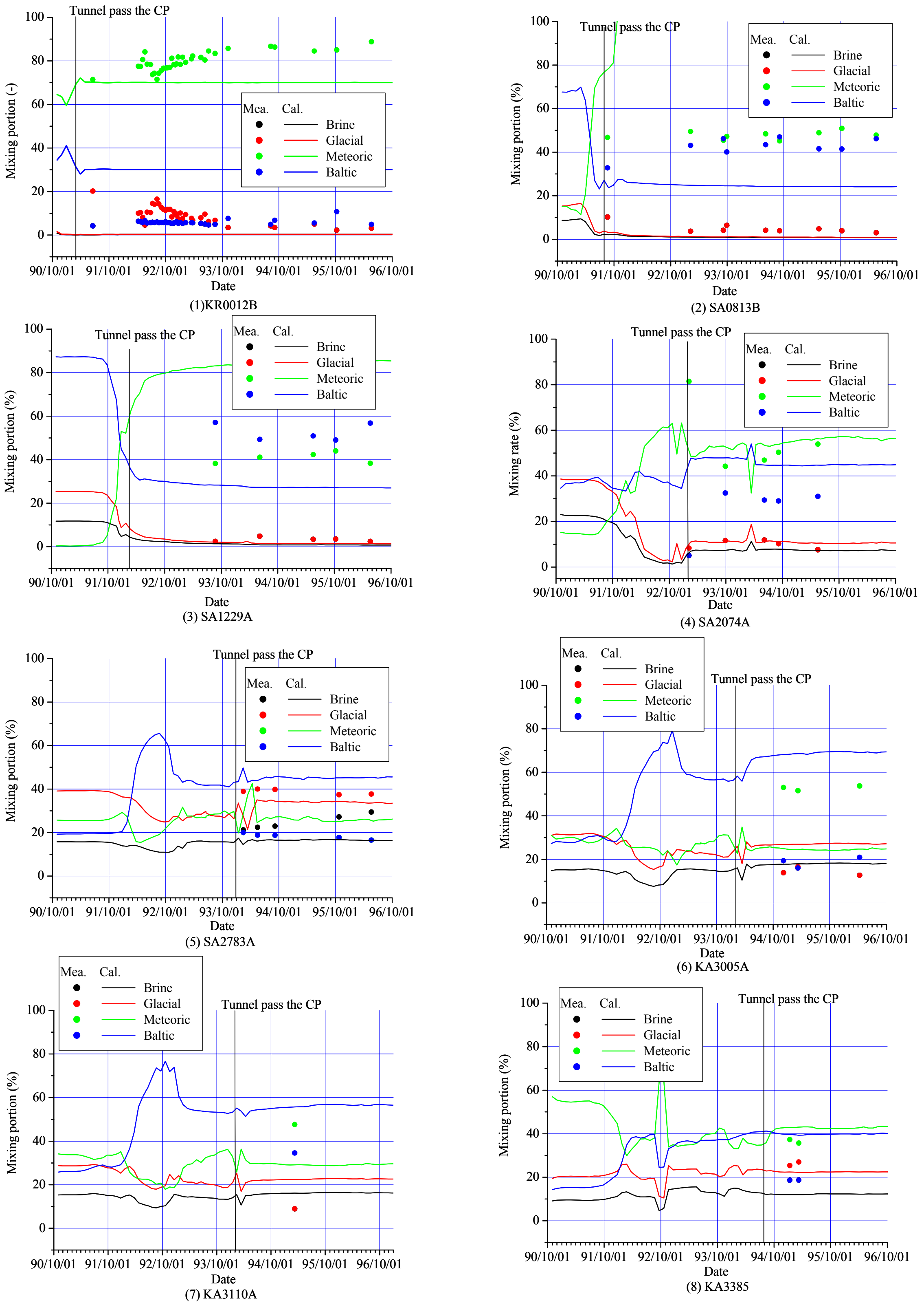
Since the replacement of groundwater in the surrounding bedrock occurred when the tunnel excavation passed the monitoring points, the groundwater movement was deduced by tunnel construction. The changes in mixing proportions were caused therefore by changes in flow due to tunnel construction.

The main features of the calculated mixing proportions at the monitoring points were deduced as follows:

- Along the access tunnel where the monitoring points were located at shallow depths, the groundwater simply flowed from the top boundary to the tunnel as expected, and the groundwater tended to be replaced by modern, fresh water (i.e. Baltic Sea and Meteoric waters). Accordingly, the mixing proportion of old water (i.e. Äspö Brine and Glacial waters) decreased. At the deeply located monitoring points which represented intersections through the HCDs, replacement by modern, fresh water still occurred, but the old water proportions remained as a few tens of percent.

- The simulated mixing portions of old waters (i.e. Äspö Brine and Glacial waters) and the sum total of modern, fresh waters (i.e. sum total of Baltic Sea and Meteoric waters) agreed with the M3 results but the ratio of modern, fresh water disagreed. Based on the simulated mixing proportions, the deeper part of the groundwater was replaced by Baltic Sea water rather than Meteoric water.

Further studies are needed to explain this inconsistency, for example, geochemical reactions, boundary conditions, local effect of sampling etc. However, focussing on the end members was useful to understand the groundwater flowpaths and the properties of the HCDs.



(1)KR0012B

(2) SA0813B

(3) SA1229A

(4) SA2074A

(5) SA2783A

(6) KA3005A

(7) KA3110A

(8) KA3385

Figure 5-38. *Simulated mixing proportions of groundwater end members at the monitored control points (Hasegawa et al., 2002).*

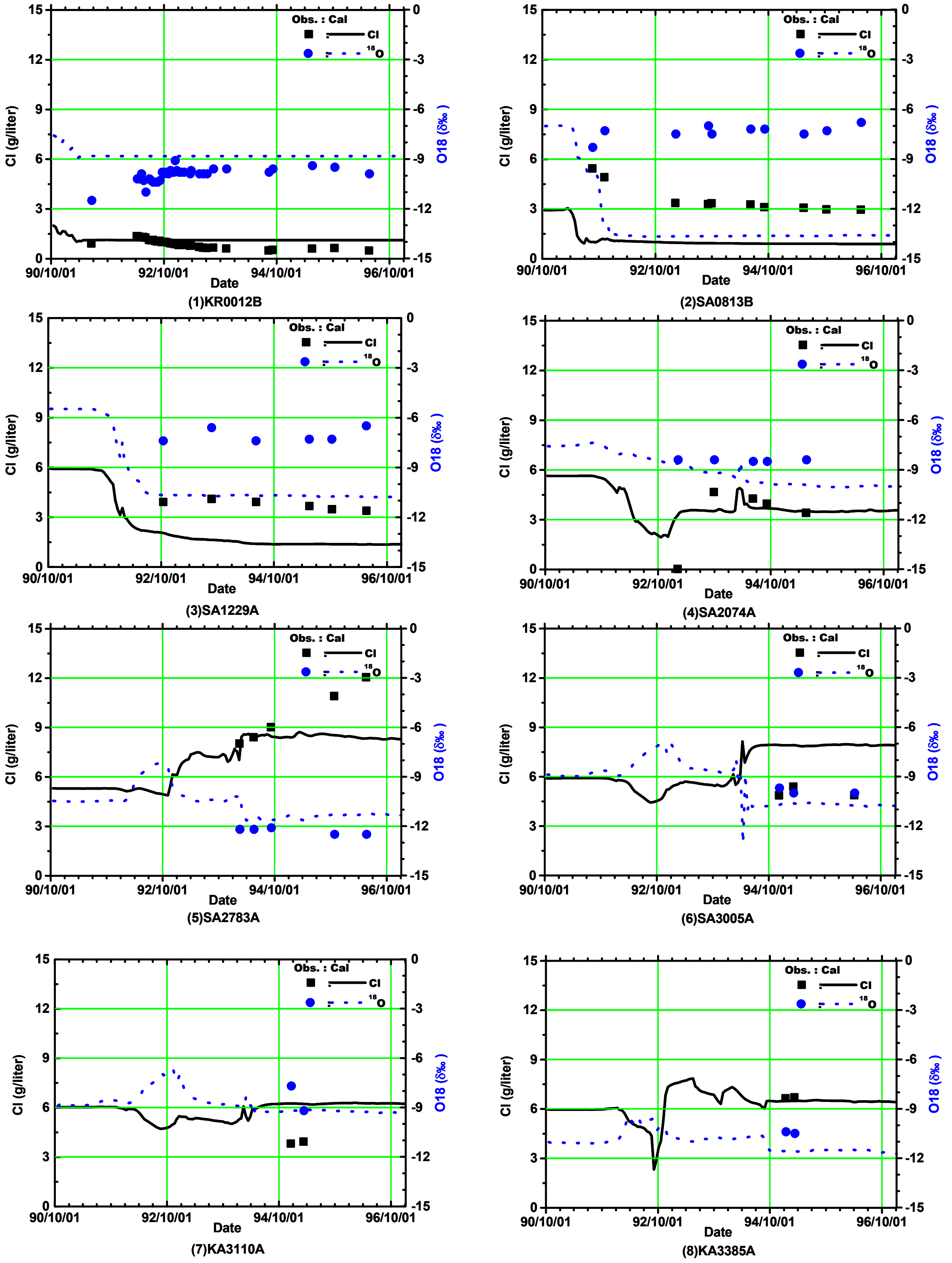


Figure 5-39. *Concentration changes of conservative tracers at the monitored control points during tunnel construction (Hasegawa et al., 2002).*

5.4.7 Enresa/UDC

Enresa/UDC constructed a not fully "3D" model, including the HCDs but not the HRDs, covering an equivalent volume of rock to most of the groups (*Fig. 5-40*). Constant properties within each HCD were assumed. See Table 4-1 for more details about the modelling approach used.

In *Figure 5-41* a comparison between measured and simulated head is shown for a few control points.

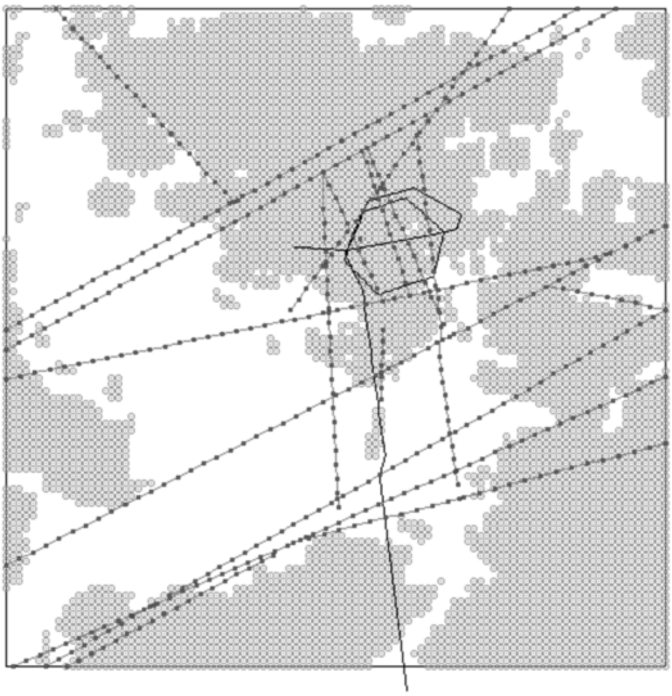


Figure 5-40. *Modelled area: ENRESA/UDC (Molinero et al., 2002).*

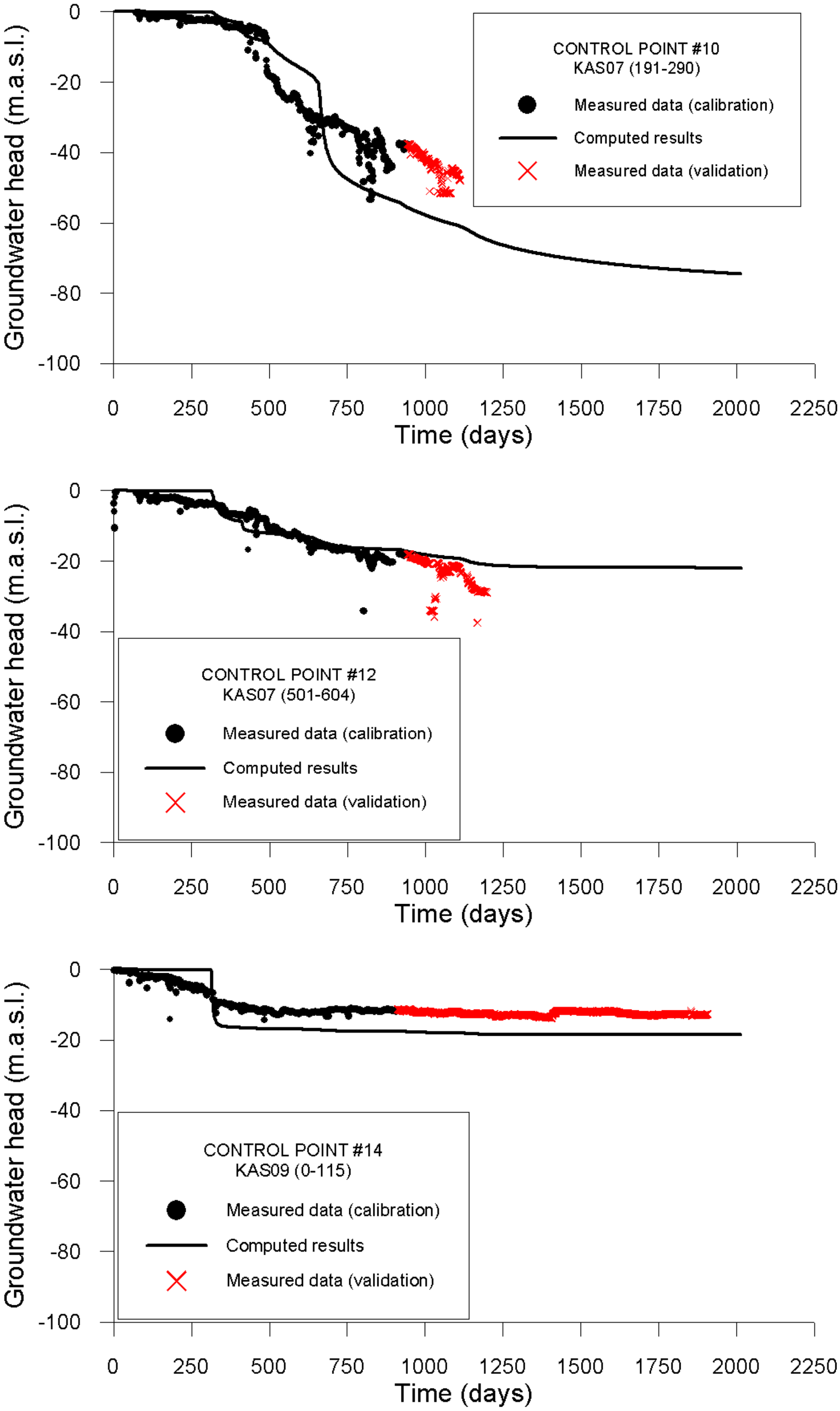


Figure 5-41. *Measured and simulated heads for a few control points: ENRESA/UDC (Molinero et al., 2002).*

Figures 5-42 to *5-45* show selected results of the modelled mixing proportions and electrical conductivity at the weirs. The major conclusions were:

- Only minor changes of HCD properties were needed and the transport parameters remained unchanged. The piezometric heads and the concentrations of chlorine and ^{18}O were all considered to show agreement with the measured values.
- The uncertainty in the initial conditions was considered to be the most important source of uncertainty.

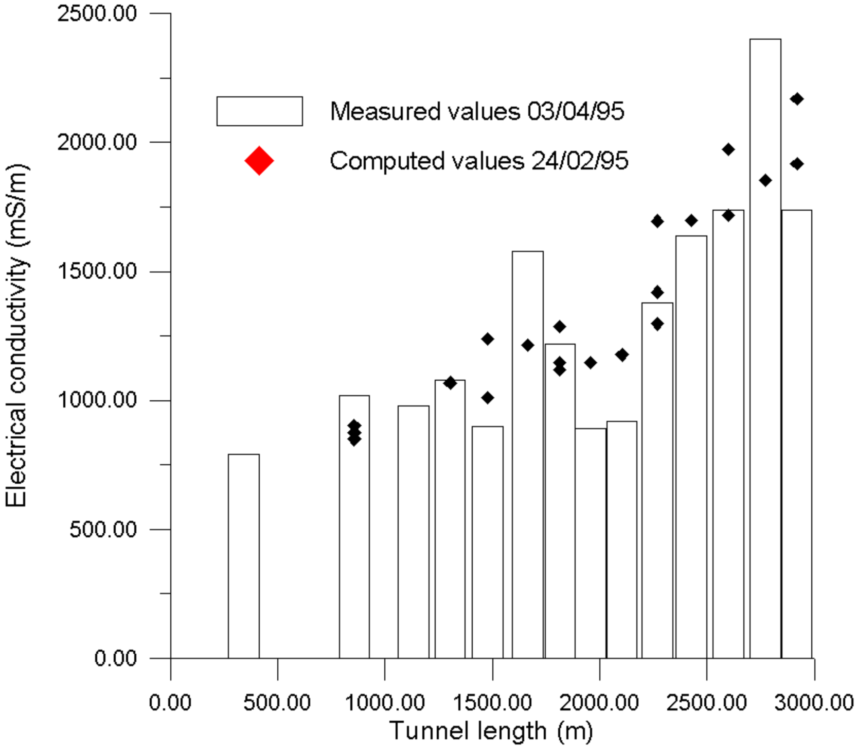


Figure 5-42. *Simulated and measured values of electrical conductivity of the waters measured at the weirs in the tunnel (Molinero et al., 2002).*

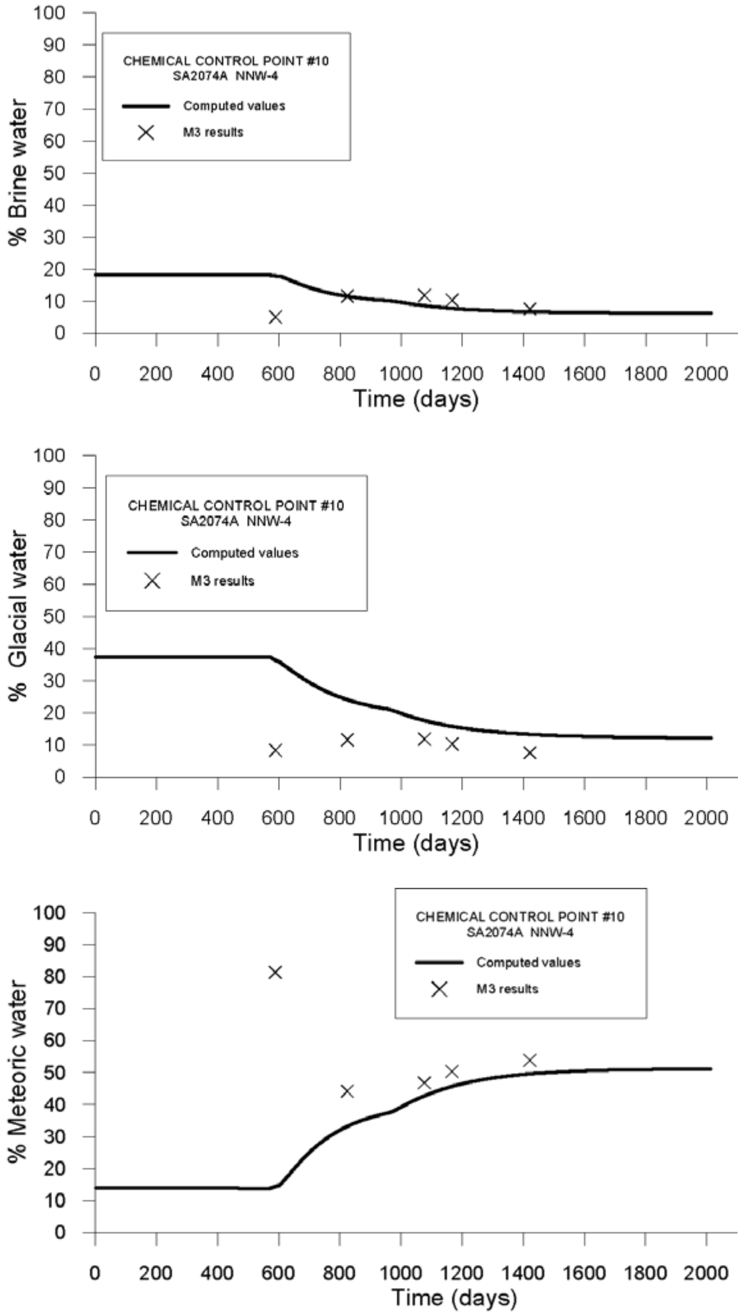


Figure 5-43. *Simulated and measured mixing proportions (based on M3) for borehole SA 2074A (Molinero et al., 2002).*

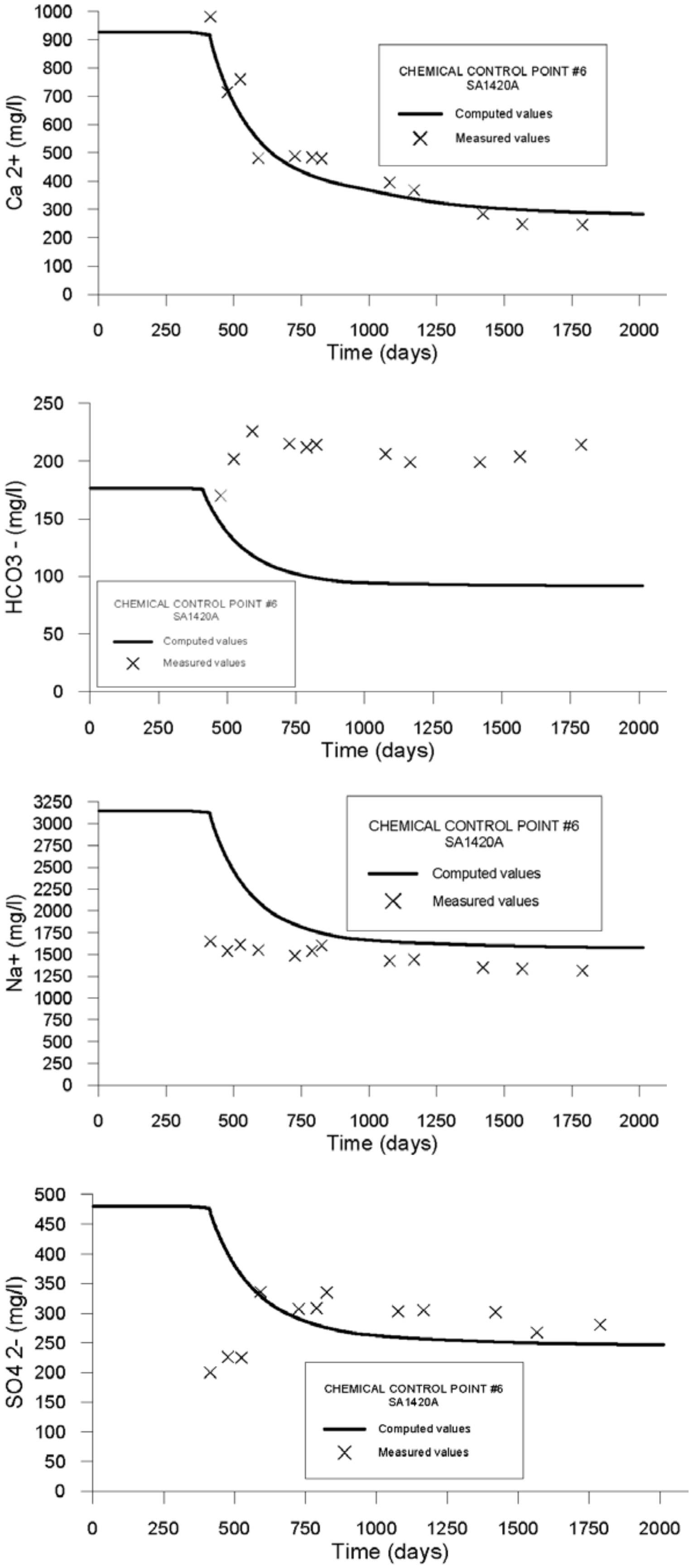


Figure 5-44. *Comparison between computed and measured concentrations of* Ca^{2+}, HCO_3^-, Na^+ *and* SO_4^{2-} *at borehole SA1420A (Molinero et al., 2002).*

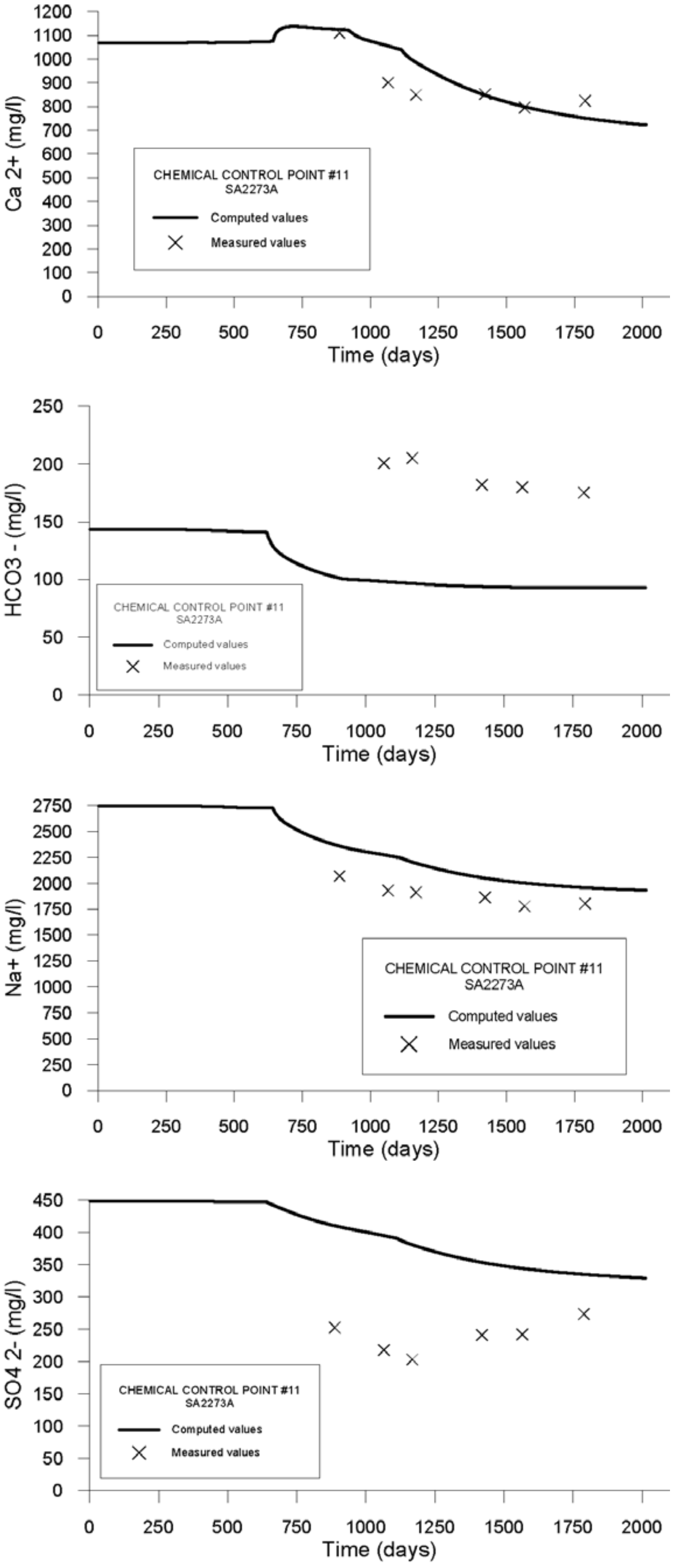


Figure 5-45. *Comparison between computed and measured concentrations of Ca^{2+}, HCO_3^-, Na^+ and SO_4^{2-} at borehole SA2273A (Molinero et al., 2002).*

5.4.8 JNC/Golder

JNC/Golder constructed a fully 3D model, including the HCDs and the HRDs, covering an equivalent volume of rock to most of the modellers (*Fig. 5-46*). Constant properties within each HCD were used. The HRDs were constructed from a stochastic Discrete Fracture Network (DFN) (*Fig. 5-47*). See Table 4-1 for more details about the modelling approach used.

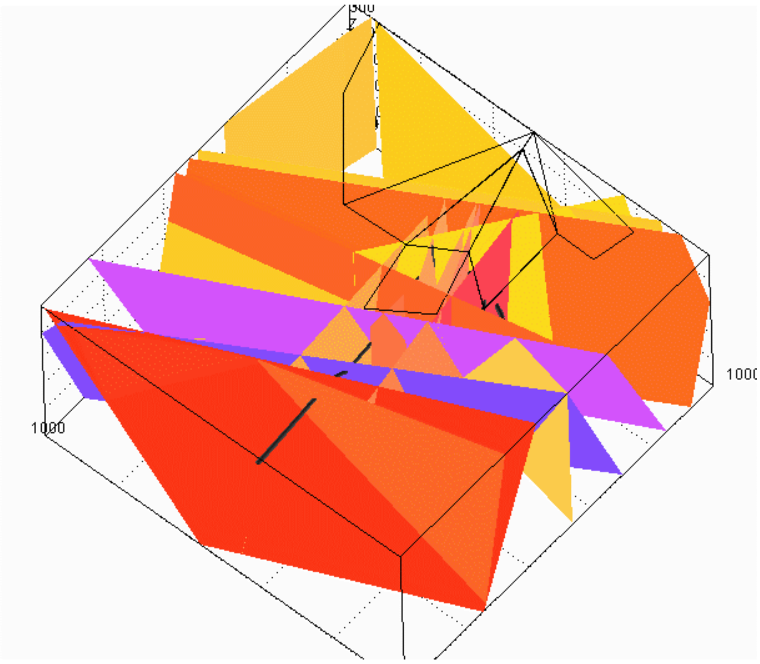


Figure 5-46. *Modelled area; structural model of the HCDs: JNC/Golder (Dershowitz et al., 2002).*

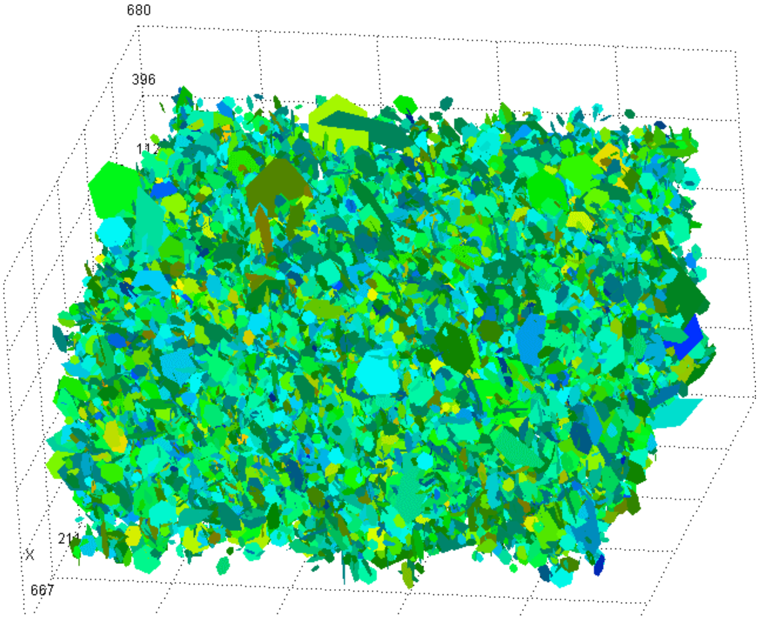


Figure 5-47. *Modelled area; background fracturing: JNC/Golder (Dershowitz et al., 2002).*

The modelling strategy by JNC/Golder was the most ambitious of all the groups. The purpose of the modelling was defined as demonstrating the value of geochemical data for construction and validation of hydrogeological and pathway models. To address these objectives, the modelling was undertaken in three separate stages:

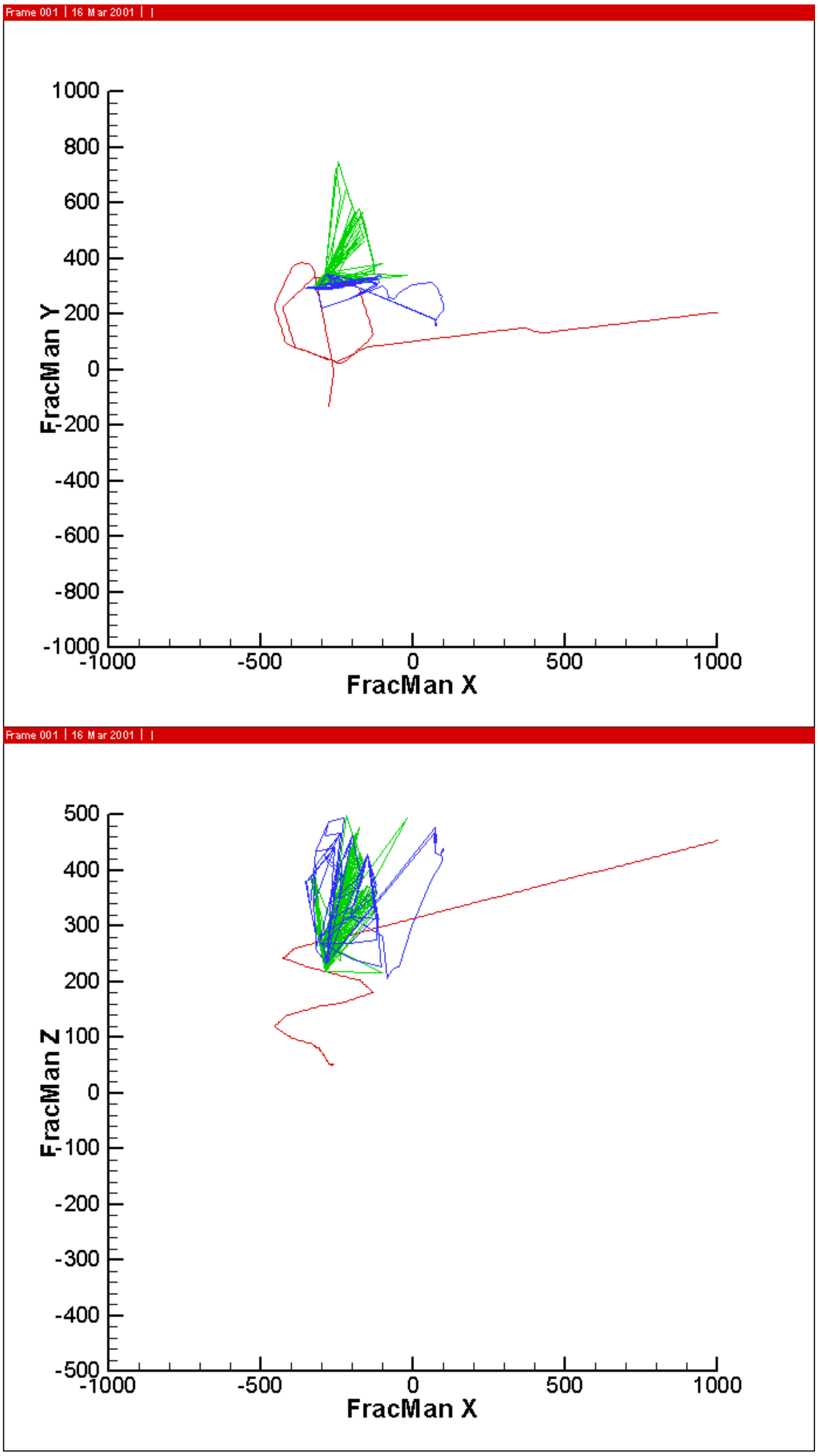
- Stage 1 Calibration and prediction based on hydrological data only (April 1999);
- Stage 1.5 Improve the calibration and prediction for Stage 1 based on hydrological data only (October 1999);
- Stage 2 Update based on geochemical data; repeat predictions (October 1999);
- Stage 3 Complementary analysis to address uncertainty issues (November 2000).

The flow paths were analysed using a two-stage approach to generate the source locations of the groundwaters flowing into the monitoring sections:

1. Determine the spatial location of the pathways
2. Determine the distance travelled along each pathway each month using the head solution along each path. This head solution was updated every 30 days based on the transient finite element solution.

JNC/Golder also tested different approaches to locate pathways: a) PAWorks graph theory (based on finding pathways up-gradient using rules for flow weighting) and b) PAWorks Particle Tracking Search (at each intersection an individual particle is assigned to the up-gradient pipes stochastically, the weighting of each pipe being in proportion to the flow). The latter method was developed because of a lack of accurate computation to determine the proportion of flow coming from each location, and also specifying the pathway coordinates based on a single flow simulation.

The flow paths for the two methods are illustrated in *Figure 5-48*. The particle-tracking algorithm resulted in more clustered pathways and more pathways towards the east. This occurred because the flow was preferentially along the large-scale features and hence most of the particles followed these paths. Conversely, although the particle-tracking algorithm shared many of the same paths as the up-gradient algorithm, it also included some of the less likely pathways. The pathways also showed the effect of the changing head distribution with time, which could be incorporated into the particle tracking results.



Blue = graph theory algorithm
Green = particle tracking algorithm

Figure 5-48. *Flow paths to monitoring section SA2074A (Control Point 4) based on a graph theory algorithm and particle tracking algorithm pathways (2-D) (Dershowitz et al. 2002).*

Figures 5-49 to *5-51* show selected results of the modelled mixing proportions. The following conclusions were drawn:

- Calibration of heads, using a well-defined geological model as the starting point, provided a reasonable estimate of the local connectivity of the system. However, the time dependence of the flows into the tunnel was generally not well modelled.

- The inclusion of hydrogeochemical data allowed a much better fit to the time dependence of the model. The data also highlighted where additional connections were required to increase the connectivity to a specific area of the model. Inclusion of such features improved the head calibration, as well as the chemistry fit. However, the results proved to be highly sensitive to the methodology used to spatially locate the initial end members, and to a lesser extent to the choice of chemical components. As the Äspö site is dominated by the large-scale features, it was necessary to use these large-scale features as the dominant influence on the chemistry. The Kriged grid of chemistry locations, combined with a linear interpolation scheme to compute the chemistry between the grid points, did a poor job of calculating the chemistry of the inflows. It was believed that the reason for this poor calibration was that the Kriging and interpolation scheme did not incorporate the geology of the model into the interpretation.

- Because this staged approach was very general, it was considered applicable to other potential repository sites. The staging was advantageous because it necessitated constructing a good geology based Discrete Fracture Network (DFN) model of the site prior to calibration. Without such a structure for the DFN, the problem would have been poorly constrained and the calibration non-unique. A unique calibration is probably unlikely to be obtained in practice, but the staged approach enabled the dominant features to be well replicated.

- The head and geochemical data provide differing constraints on the model. Head data were critical, and were recommended to calibrate the model prior to geochemical input. The reasons for using the head data first were that this information was considered less ambiguous. The time dependent head information was dominated by local connectivity and transmissivities as the tunnel section was being constructed, and by the regional connectivity and boundary conditions later on. It was reasoned, therefore, that if the original fracture model accurately reflected the major connectivity, the missing connectivity (e.g. the 'Mystery Feature') and boundary conditions could be calibrated fairly successfully.

- The hydrogeochemical information provided the only real constraint (or validation) on the source location of waters predicted by a model. This calibration provided information, like the head data, on whether a major connection was missing. However, in common with the head calibration, it relied on having a good underlying DFN model that already replicated most of the major hydraulic structures.

- Additionally, hydrogeochemical data were used to calibrate transport apertures and storage affects. These effects are difficult to calibrate using solely time dependent head measures at tunnel sections.

- The Äspö Task 5 modelling had access to a wide range of data and generally the quality of these data was very high. JNC/Golder indicated that the staged approach was advantageous to allowing a systematic assessment of the modelling success. The area where the data could possibly be improved for future performance assessment of repository sites was related to the choice of locations. Generally, the aim of the model validation was to indicate whether the model correctly replicated the overall response on the groundwater system, while still reproducing more local effects. At Äspö the tunnel was a major influence on the groundwater system. It was considered important, therefore, to ensure that any model used for Performance Assessment (PA) should correctly replicate these affects. However, the groundwater and pressure regime immediately adjacent to the tunnel was also influenced by the effect of grouting behind the tunnel lining (e.g. reduced inflows into tunnel and head drop across the tunnel lining). For a regional scale model these effects would be difficult to include and would not improve understanding of the overall system response. Therefore, where possible, data and calibration locations should be beyond the zone of influence of these activities.

- Hydrogeochemical measurements prior to tunnel excavation produced a more accurate representation of the *in situ* chemistry distribution, as the tunnel construction was seen to markedly affect the flow regime. Therefore, more early time measurements are advantageous (although difficult to obtain in practice). For the calibration process, hydrogeochemical measurements distributed approximately evenly through time would have enabled the flow velocities to be more accurately calibrated. The use of measurement boreholes both within the main fracture zones, and within the background network, were useful in determining the proportion of flow occurring in the different fracture types.

The current modelling was focused on the heads and chemistry measured over several years. For PA the time scale is much longer, typically thousands to hundreds of thousands of years. It was pointed out that the usefulness of this modelling to longer time scales should be considered. Tunnel construction will likely involve the largest head changes to occur throughout a repository construction and operation. Hence, a good fit to head and hydrogeochemical responses will give confidence in the connectivity and transmissivity of the DFN. Prediction of long-term head distributions is more difficult, as the boundary conditions that should be applied to the model are poorly defined over longer time frames. However, this is a deficiency of future knowledge, rather than a deficiency of the DFN model. Potentially, the greater deficiency is the lack of information on the hydrogeochemistry during tunnel/repository resaturation. It is important to collect hydrogeochemical information over a sufficient area to account for longer-term inflows from more remote locations. These inflows, if of differing density and chemistry, may affect the steady state pressure distribution, and possibly chemical reactions within the rock mass adjacent to the tunnels.

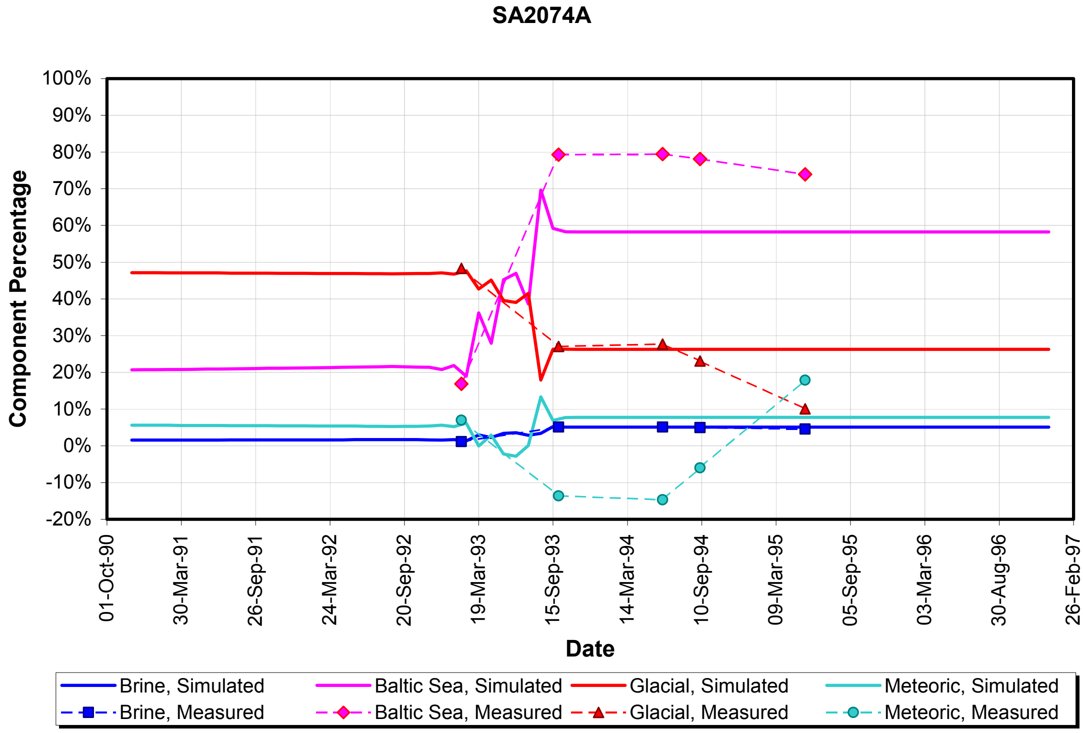


__Figure 5-49__ Control Point SA2074A: Geochemical inflows for 4 end members, based on the 7 component model; Final Model (3). Negative values are due to the least-square method to calculate the 4 end members from the 7 components. (Dershowitz et al., 2000).

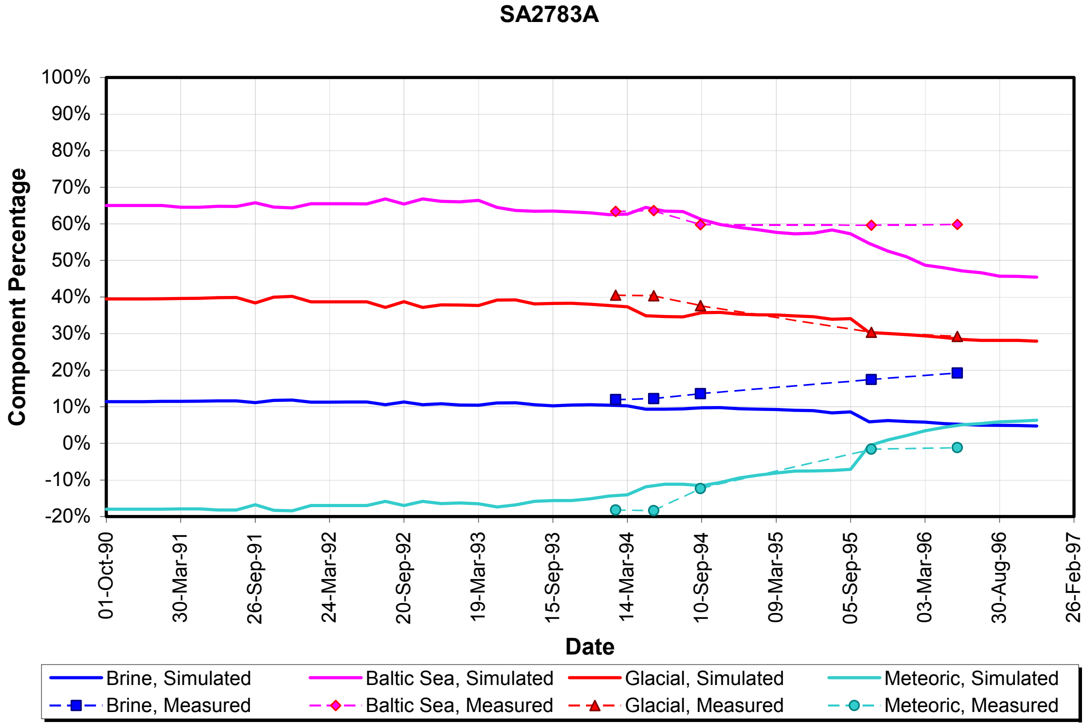


__Figure 5-50.__ Control point SA2783A: Geochemical inflows for 4 end members, based on the 7 component model; Final Model (3). Negative values are due to the least-square method to calculate the 4 end members from the 7 components. (Dershowitz et al., 2000).

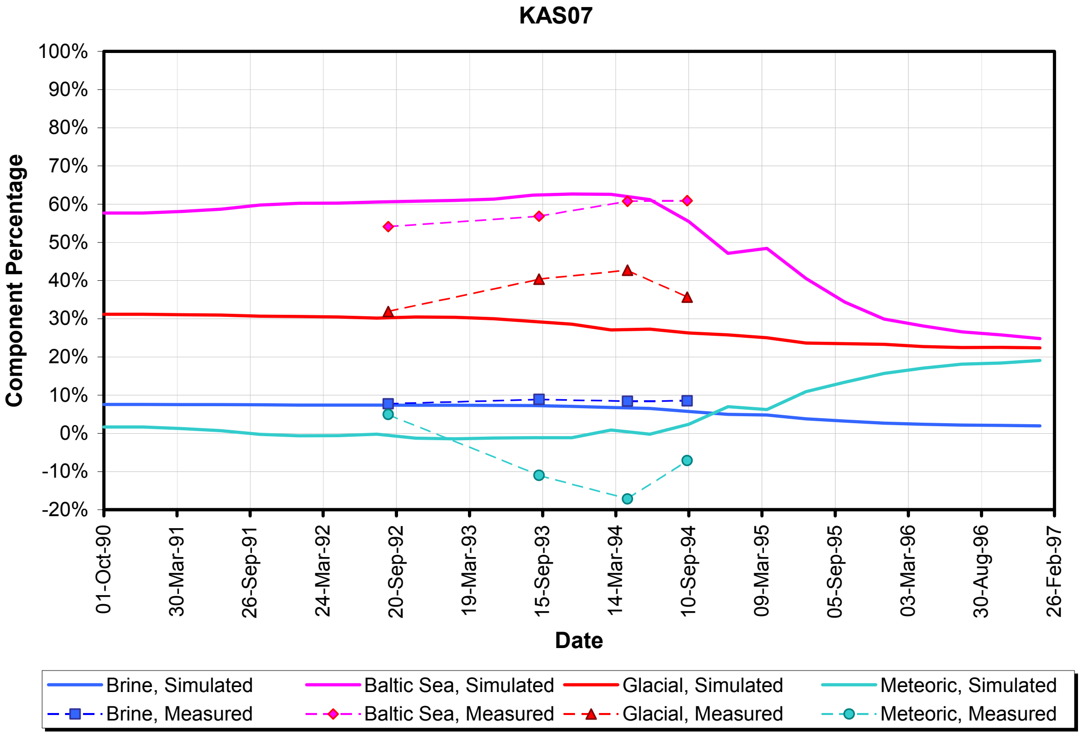


Figure 5-51. *Control point KAS07: Geochemical inflows for 4 end members; Final Model (3) (Dershowitz et al., 2002).*

5.4.9 Posiva/VTT

Posiva/VTT constructed a fully 3D model, including HCDs and HRDs, covering an equivalent volume of rock to most of the modellers (*Fig. 5-52*). The transmissivities and flow porosities of the HCDs were assumed to be depth dependent (i.e. decreasing values with depth). Constant properties within each HRD were assumed; for the HDRs dual porosity was assumed. See Table 4-1 for more details about the modelling approach used.

Flow paths were modelled to a number of control points (see *Figs. 5-53 and 5-54*).

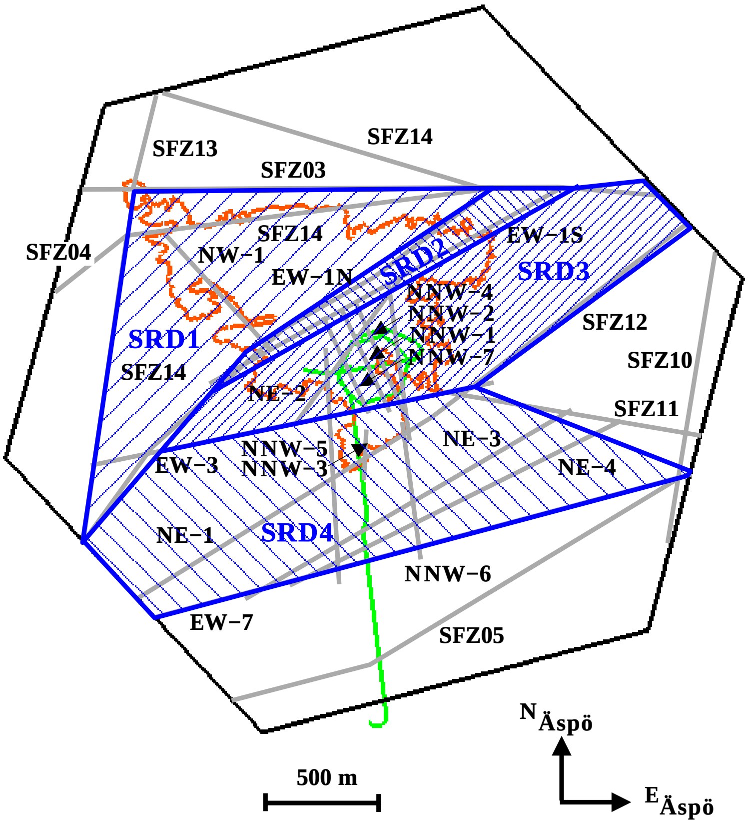


***Figure 5-52.** Modelled area with HCDs and HRDs (referred to as SRD:s in the figure): Posiva/VTT (Luukkonen and Kattilakoski, 2002).*

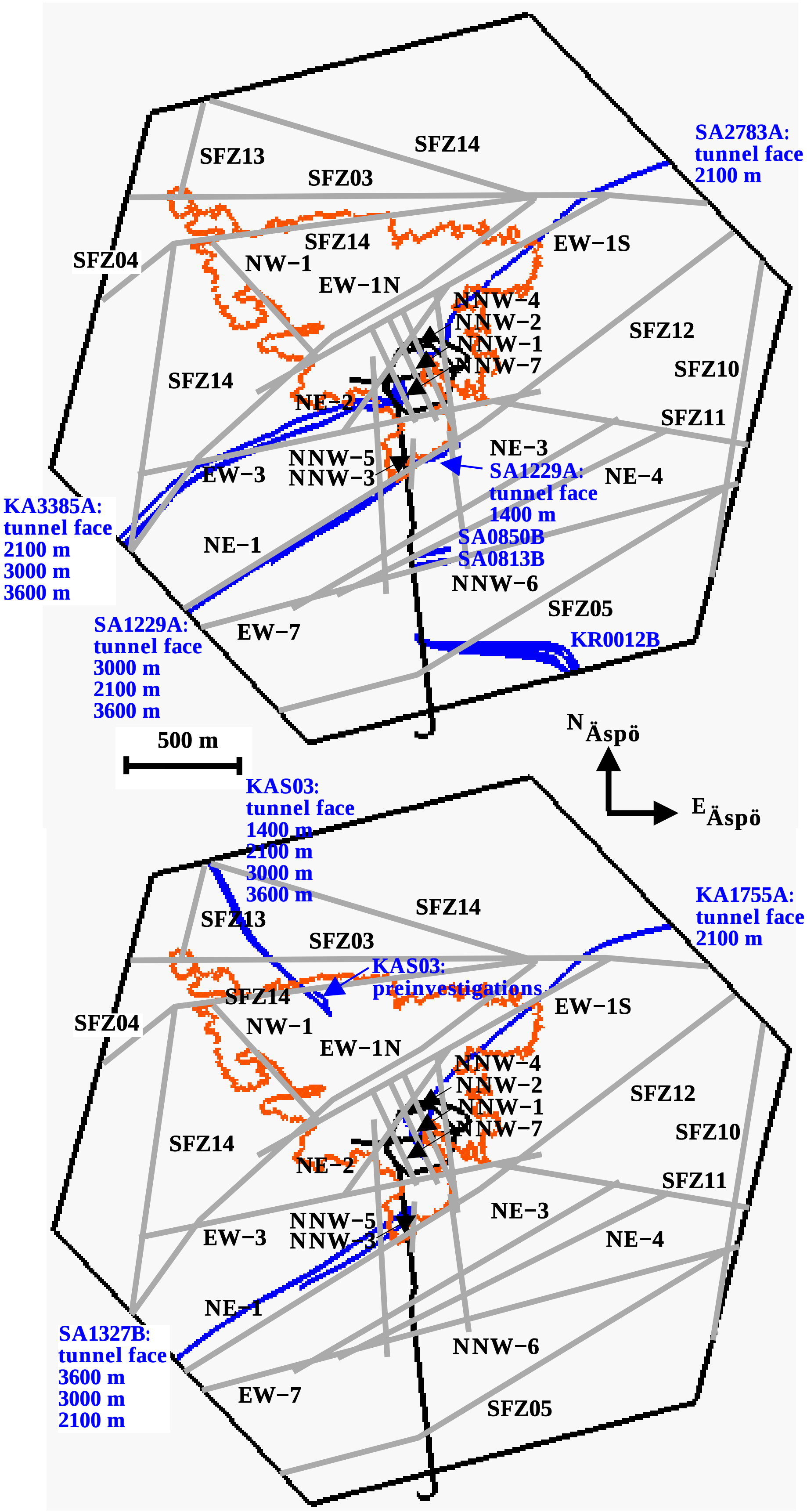


Figure 5-53. *Projections of flow paths to the control points on a horizontal plane. The coastline of the Äspö island, the fracture zones at the surface and the model boundaries are also shown: Posiva/VTT (Luukkonen and Kattilakoski, 2002).*

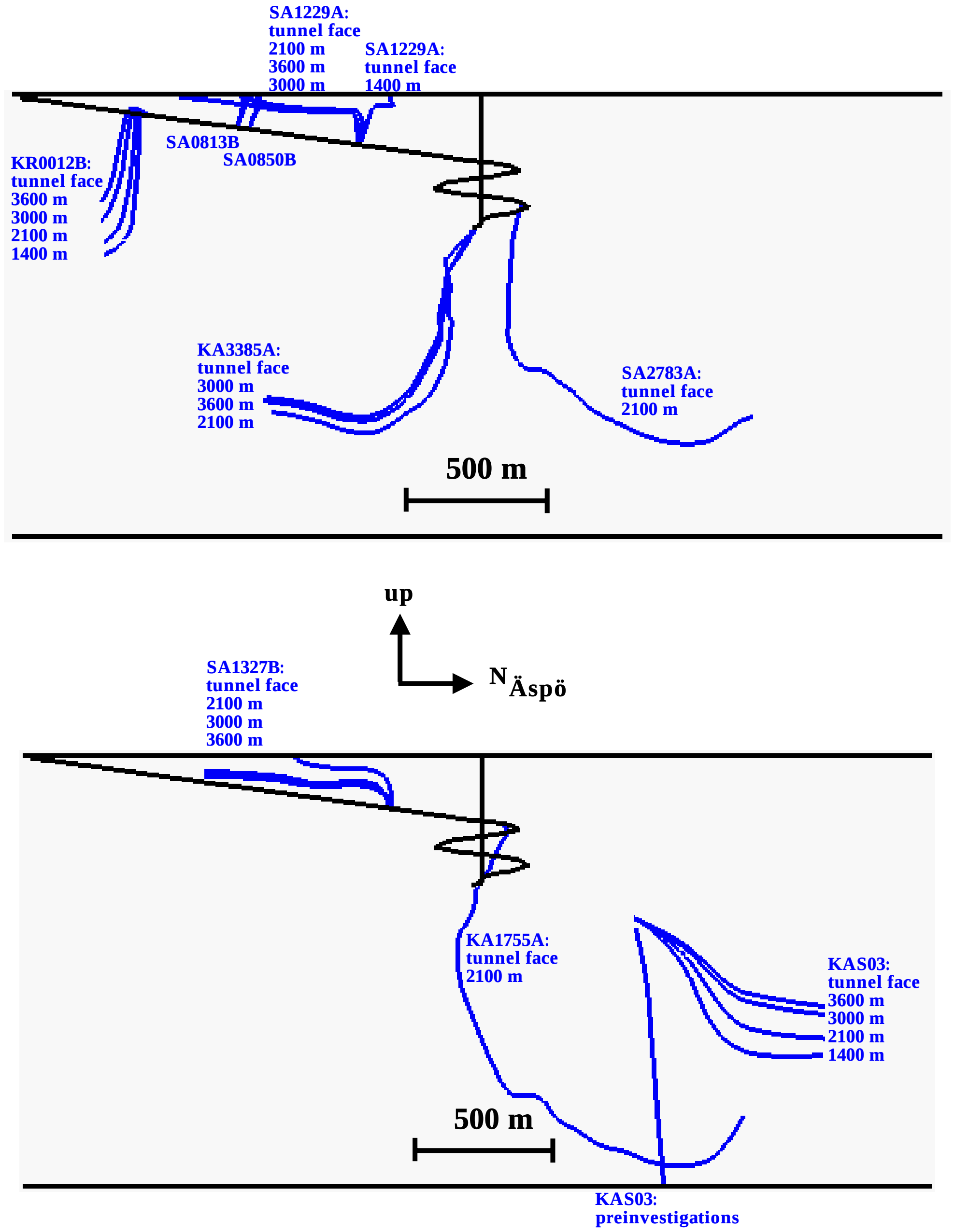


Figure 5-54. *Flow paths from a number of tunnel and external(KAS03) control points (Luukkonen and Kattilakoski, 2002).*

Figures 5-55 to *5-56* show selected results of the modelled mixing proportions. The following was concluded:

- The difficulties related to the calibration points were roughly divided between problems close to the surface and at depth. Making suitable adjustments of the surface boundary conditions and the transmissivities usually solved the shallow problems. The adjustments of the node types were generally necessary because of the 'coarseness' of the model, and the re-estimations of the transmissivity values were necessary also because of a lack of measurement values. At depth, the simulations exhibited either a systematically growing deviation from the hydrogeochemically estimated values, or hinted at an exaggerated stiffness of the hydrological model. These difficulties raised three principal questions: "are the hydrological/structural properties of the fracture zones correctly estimated at depth, are the structural relations between the fracture zones correctly defined, and is the open tunnel effect taken correctly into account in the hydrological model?"

- The confidence of the simulation results for the prediction points were not considered high. The primary reason was the amount of calibration points; only eight calibration points with time-series data were used for the model calibrations. In four of the deep control points the calibrations were not successful.

- Large volumes of the model were assumed to behave homogeneously or according to harmonic functions of depth. There were several fracture zones and hydraulic conductor domains that were not monitored during the simulations. Therefore, the current approach presented should be considered more as a feasibility study of the coupling of geochemical inverse-modelling estimations and realistic hydrological simulations. The results showed that the method is feasible, though there were some aspects in the method demanding further refinement.

- Methodological uncertainties were related to the hydrological transport of conservative mixing proportions and to the geochemical estimation of these proportions. In the exercise the distribution of each reference water type within the model had to be simulated in a separate run. Consequently, the separate simulations did not necessarily add up to 100 %. In view of the geochemical estimations as well, the uncertainties were addressed mostly to the evaluation of technical issues and deficient analytical data. The amount of available (chemically analysed) conservative parameters had a very large effect on the precision and confidence of the geochemical estimations. In all, the geochemical inverse-modelling approach was considered to be a sensitive tool if correctly used and, with a favourable amount of data, it produced truly conservative parameters (mixing proportions) that can be used as natural tracers. (*Summary Report Author's Note: It is doubtful that the calculated mixing proportions can be considered 'truly' conservative*).

- It was also noted that the dispersivity used, the extension of the fracture zones, the infiltration at Äspö island and through the sea bottom, were all uncertain.

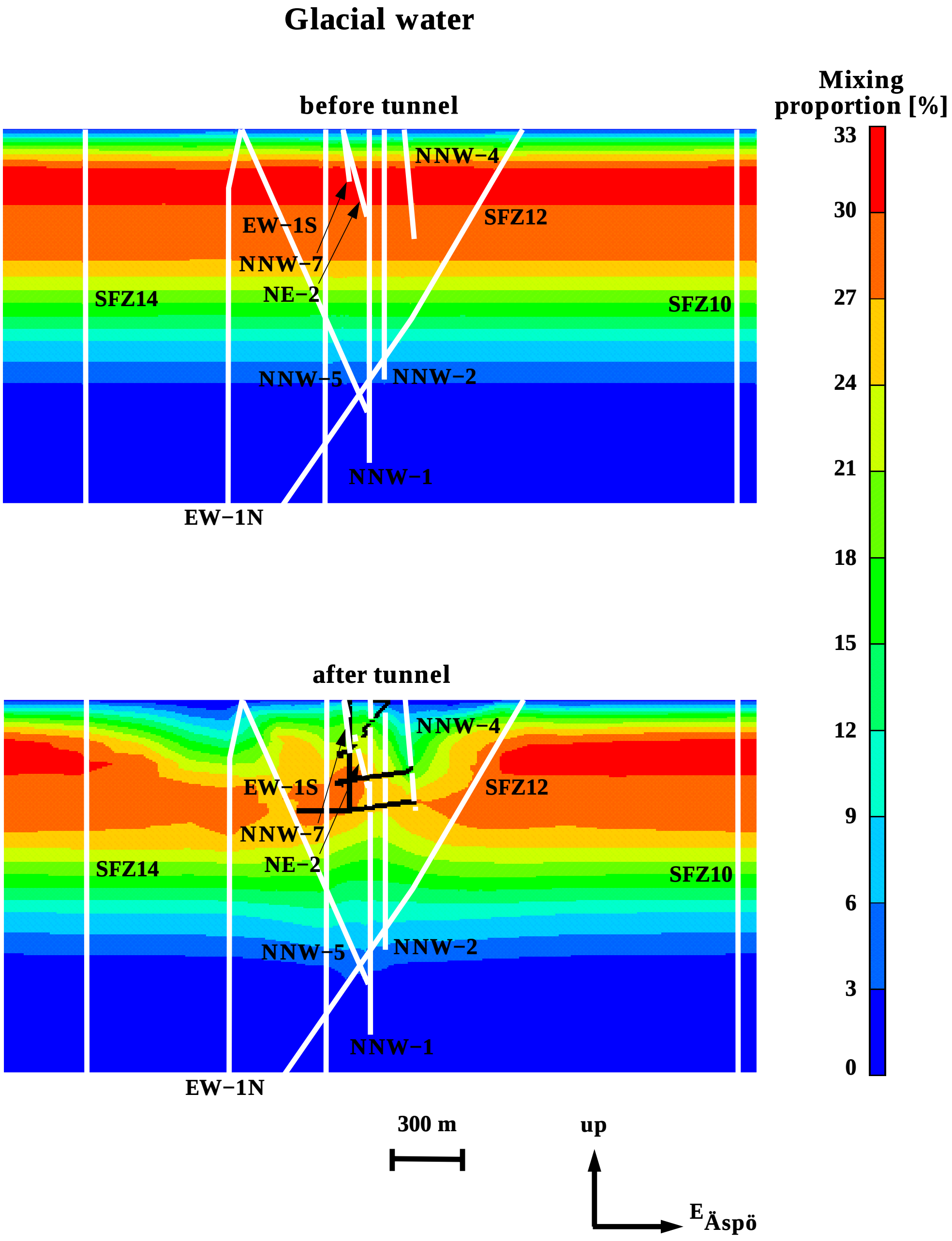


***Figure 5-55.** The mixing ratios of Glacial Water on an E-W trending cutting plane before and after the tunnel construction (Luukkonen and Kattilakoski, 2002).*

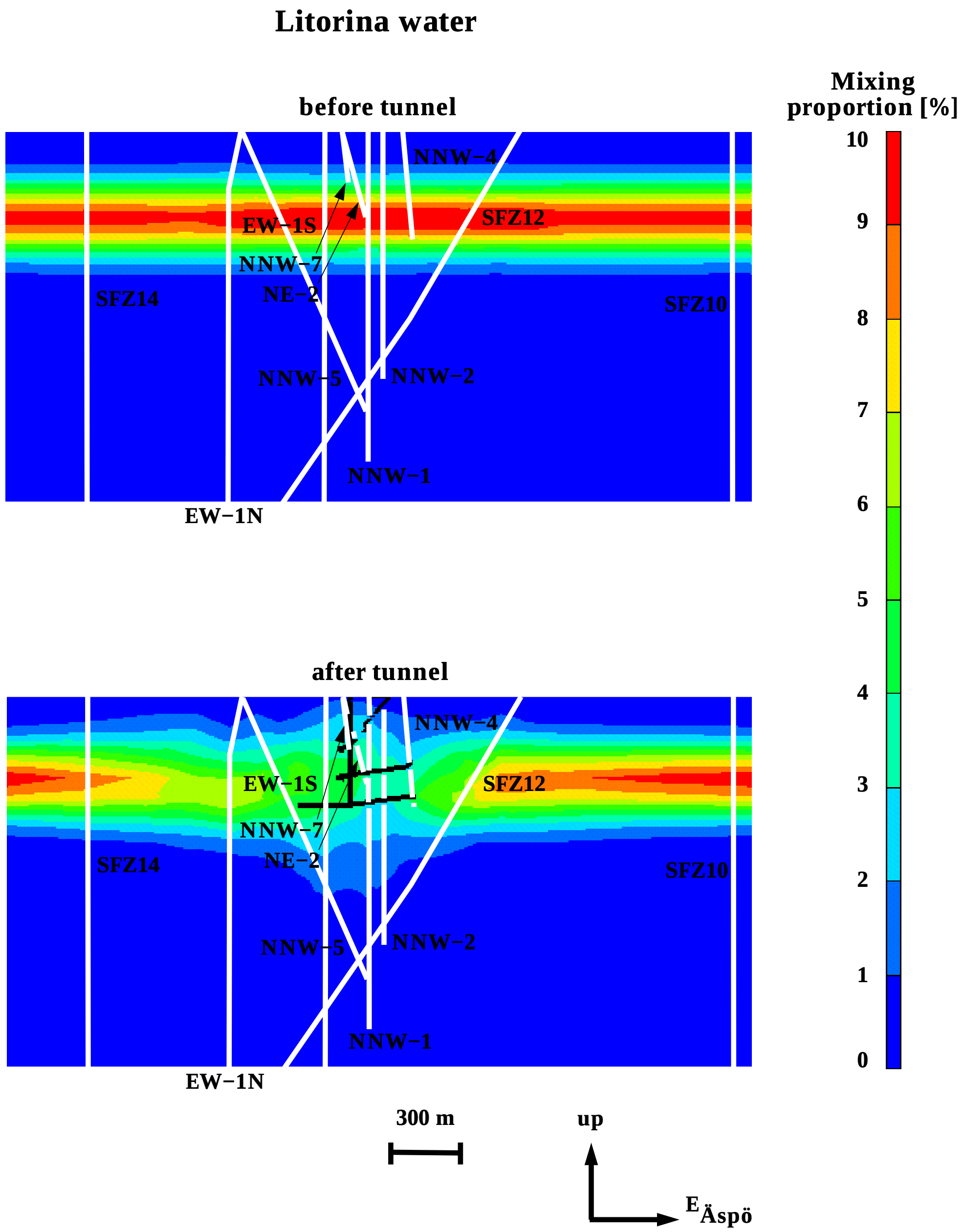


Figure 5-55 (cont.). *The mixing ratios of Litorina Water on an E-W trending cutting plane before and after the tunnel construction (Luukkonen and Kattilakoski, 2002).*

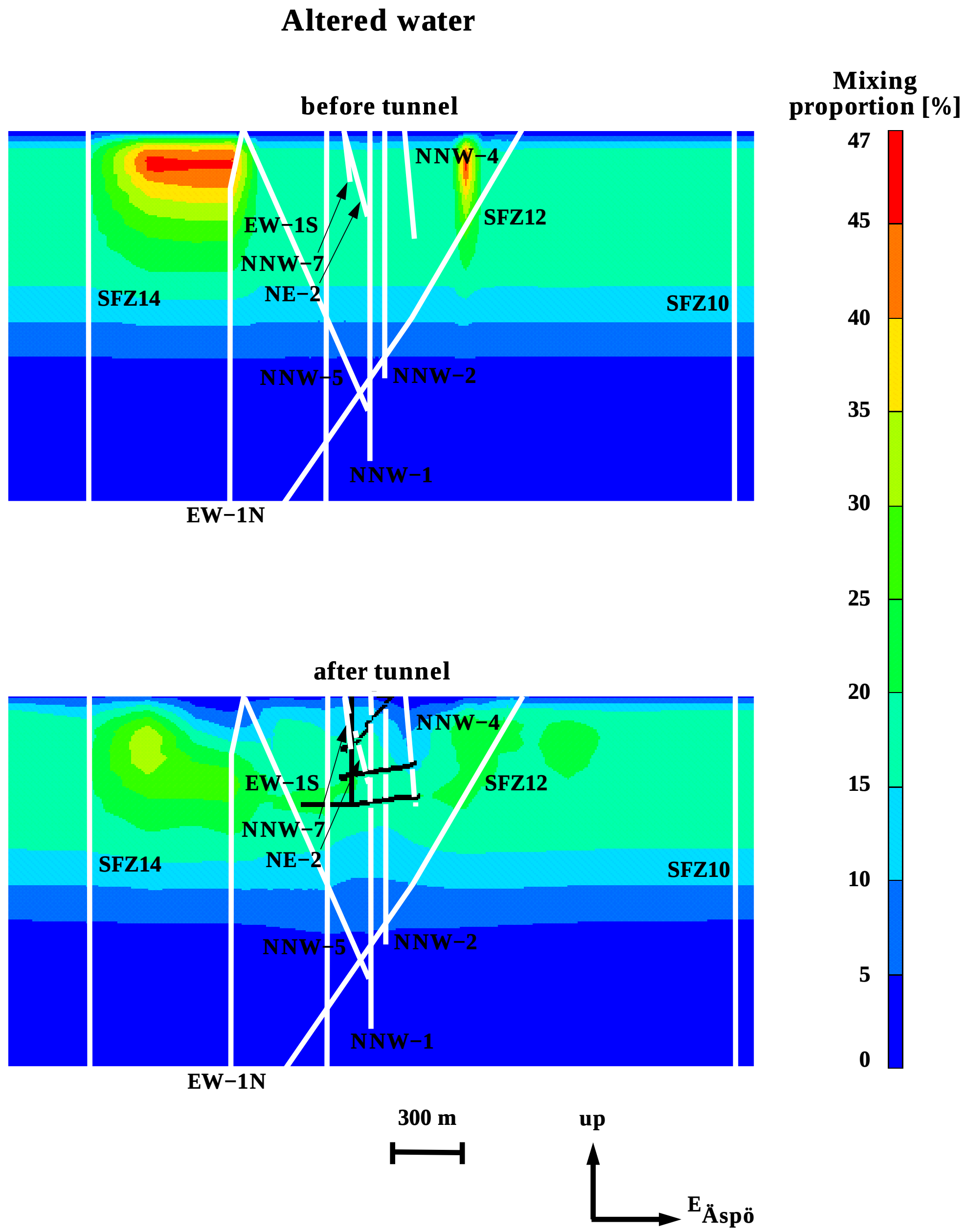


Figure 5-55 (cont.). *The mixing ratios of Altered Water on an E-W trending cutting plane before and after the tunnel construction (Luukkonen and Kattilakoski, 2002).*

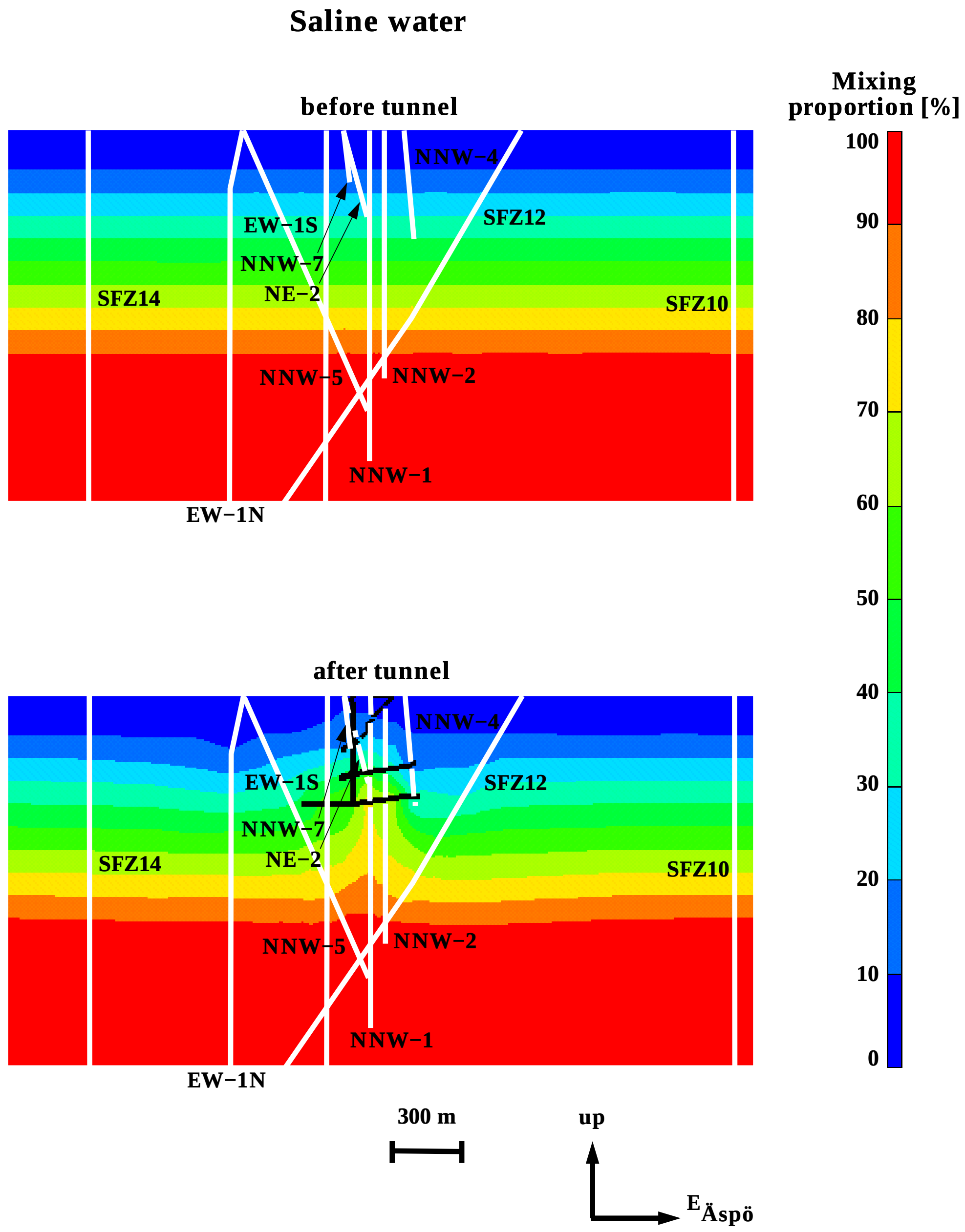


Figure 5-55 (cont.). *The mixing ratios of Saline Water on an E-W trending cutting plane before and after the tunnel construction (Luukkonen and Kattilakoski, 2002).*

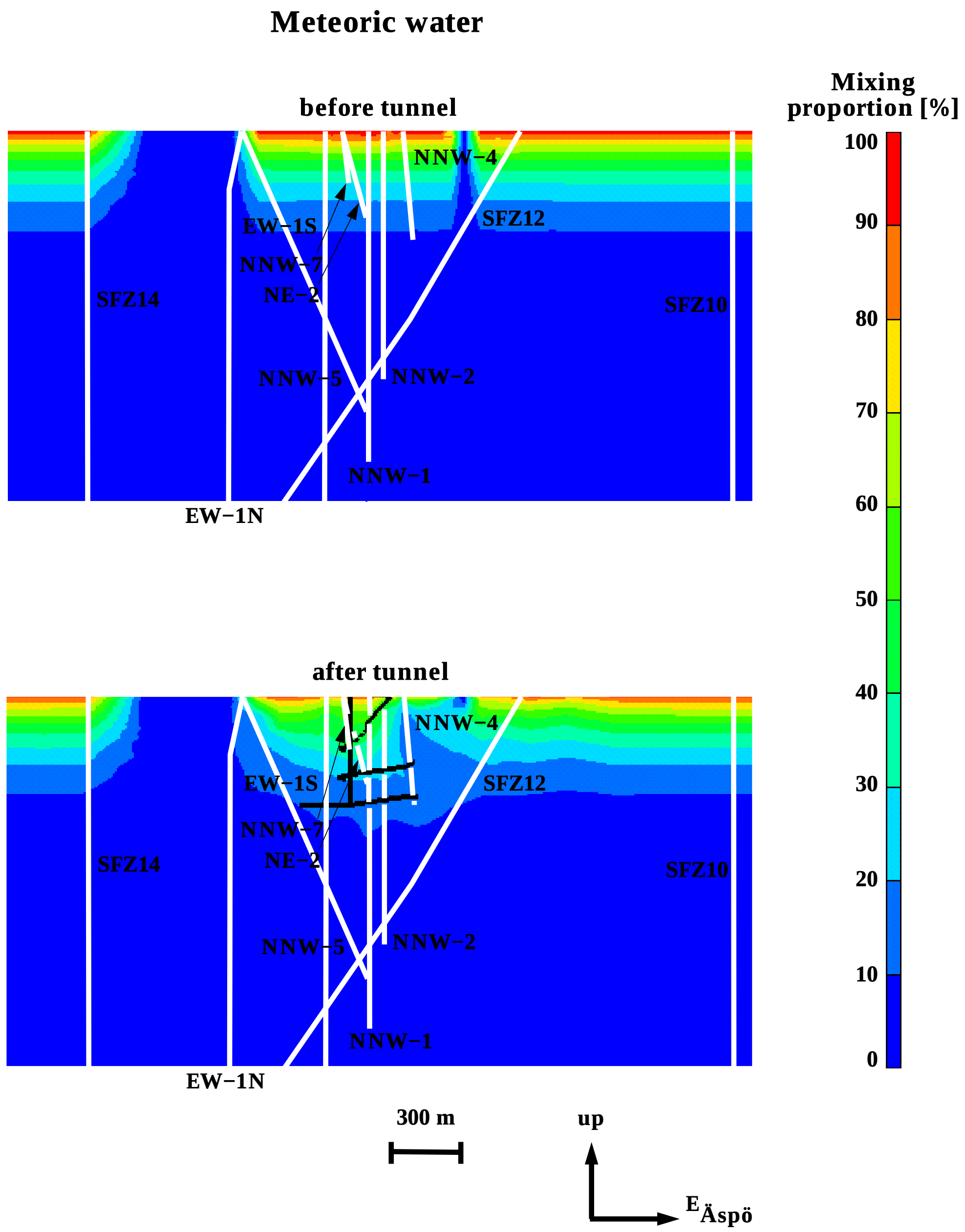


Figure 5-55 (cont.). *The mixing ratios of Meteoric Water on an E-W trending cutting plane before and after the tunnel construction (Luukkonen and Kattilakoski, 2002).*

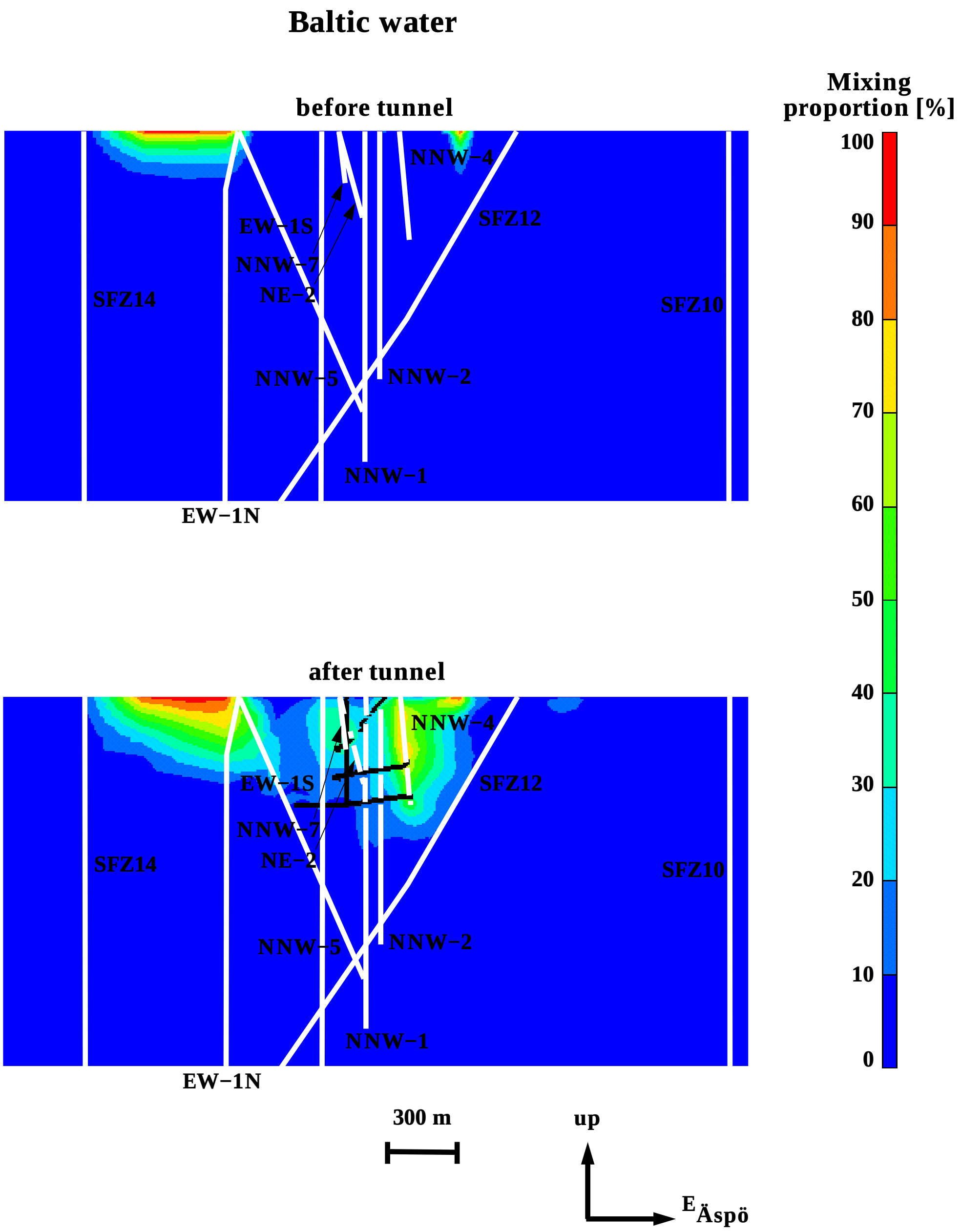


Figure 5-55 (cont.). *The mixing ratios of Baltic Water on an E-W trending cutting plane before and after the tunnel construction (Luukkonen and Kattilakoski, 2002).*

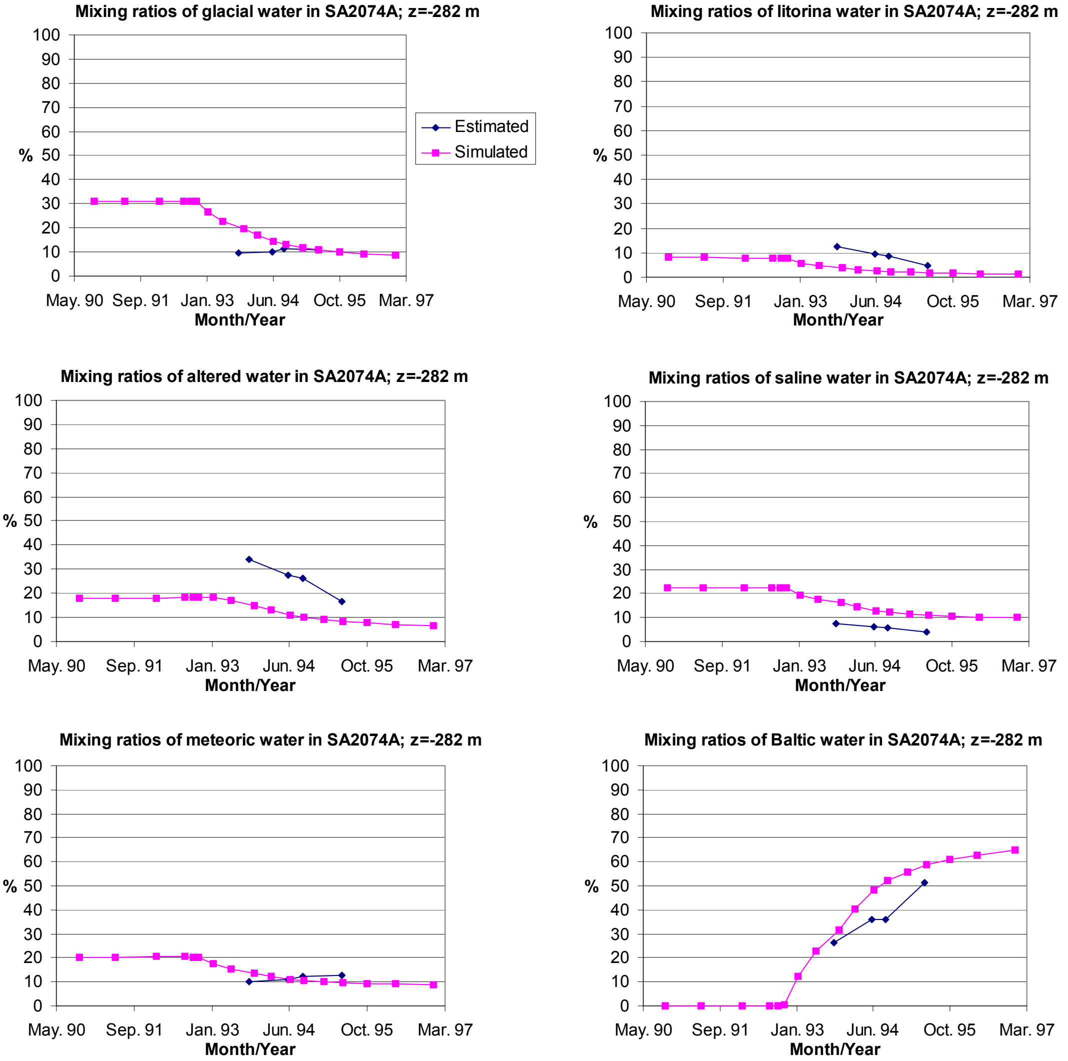


Figure 5-56. *The mixing ratios of Glacial, Litorina, Altered, Saline, Meteoric and Baltic waters in SA2074A as a function of time (Luukkonen and Kattilakoski, 2002).*

5.4.10 SKB/CFE

SKB/CFE constructed a fully 3D model, including HCDs and HRDs, covering an equivalent volume of rock to most of the modellers (*Fig. 5-57*). Constant properties within each HCD were assumed. The first model constructed used a stochastic distribution of hydraulic conductivity for the HRDs as a spatial assignment method (Model 1 in Table 4-1). In the second model, a stochastic distribution of a fracture network was used to assign properties to the cells in the model (Model 2 in Table 4-1). See Table 4-1 for more details about the modelling approach used.

Based on arguments related to the penetration of Glacial water during the last ice-age and density turn-over during the Litorina stage (after the last Glaciation), SKB/CFE assumed the hydrogeochemical conditions on the vertical boundaries (Fig. 5-57) to consist of Mixed Water High (MWH) and Mixed Water Low (MWL):

- MWH: Composition based on field data from the Laxemar borehole KLX01 (10% Baltic, 35% Meteoric, 45% Glacial and 10% Äspö Brine).
- MWL: To some degree supported by measurements from the Laxemar borehole KLX02, at depths with salinities of 1.5% (10% Baltic, 10% Meteoric, 40% Glacial and 40% Äspö Brine).

Flow paths were modelled to a number of control points (*Figs. 5-58 and 5-59*). The flow paths in Models 1 and 2 were similar, although the spread of the simulated flow paths was greater in Model 2.

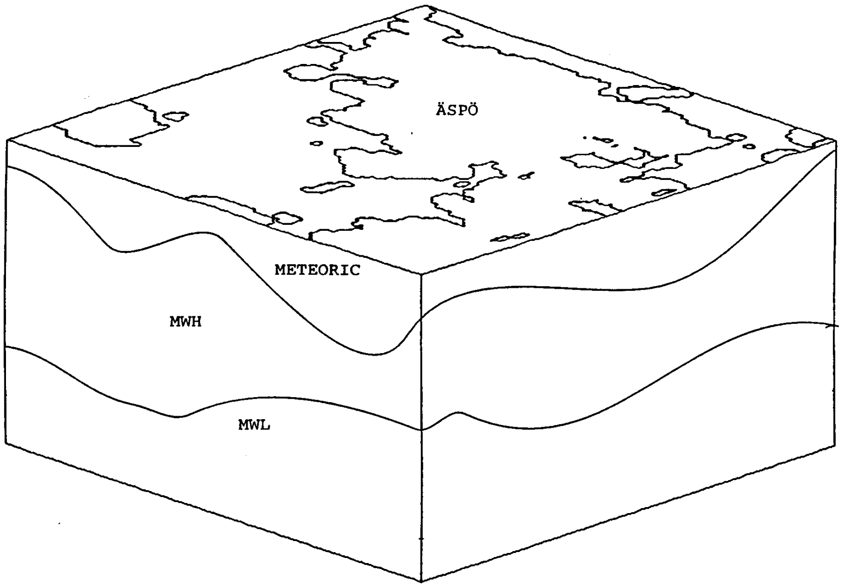


Figure 5-57. *Modelled area also indicating types of chemical boundary conditions used: SKB/CFE (Svensson et al., 2002).*

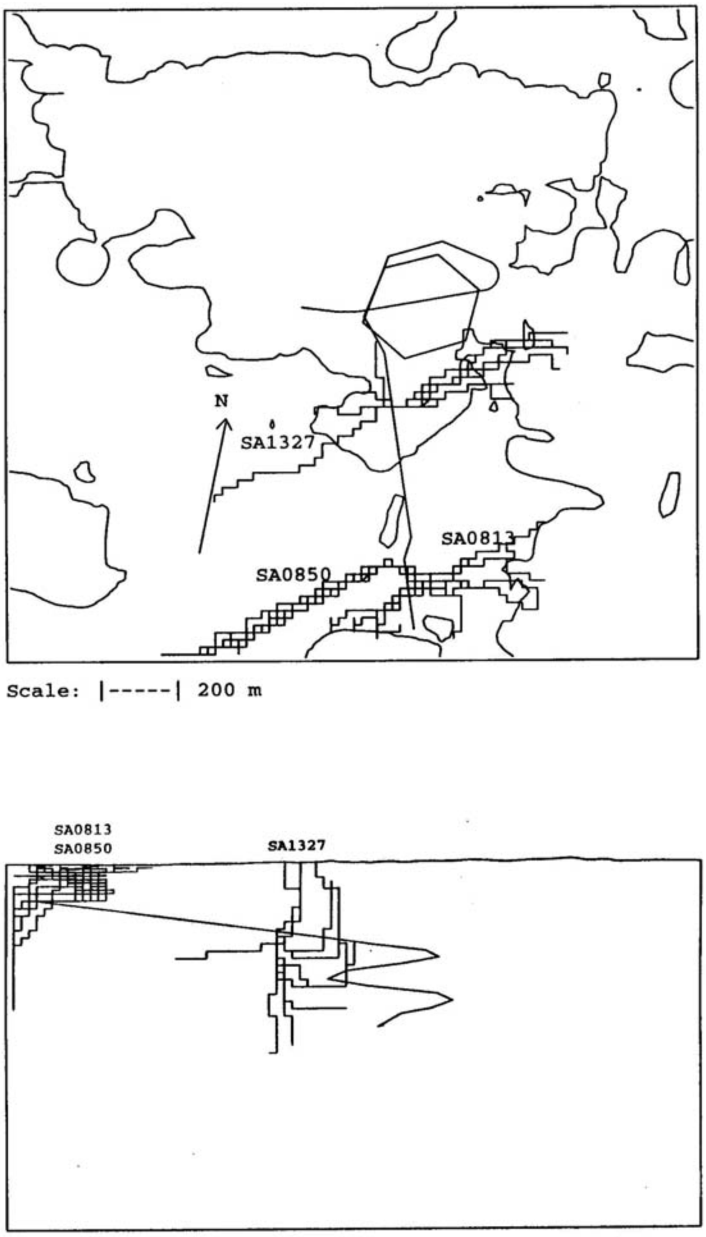


Figure 5-58. *Flow paths for water at control points SA0813, SA0850 and SA1327. Horizontal view (top) and view from east (bottom). Tunnel front at 2 100 metres (Model 2). SKB/CFE (Svensson et al., 2002).*

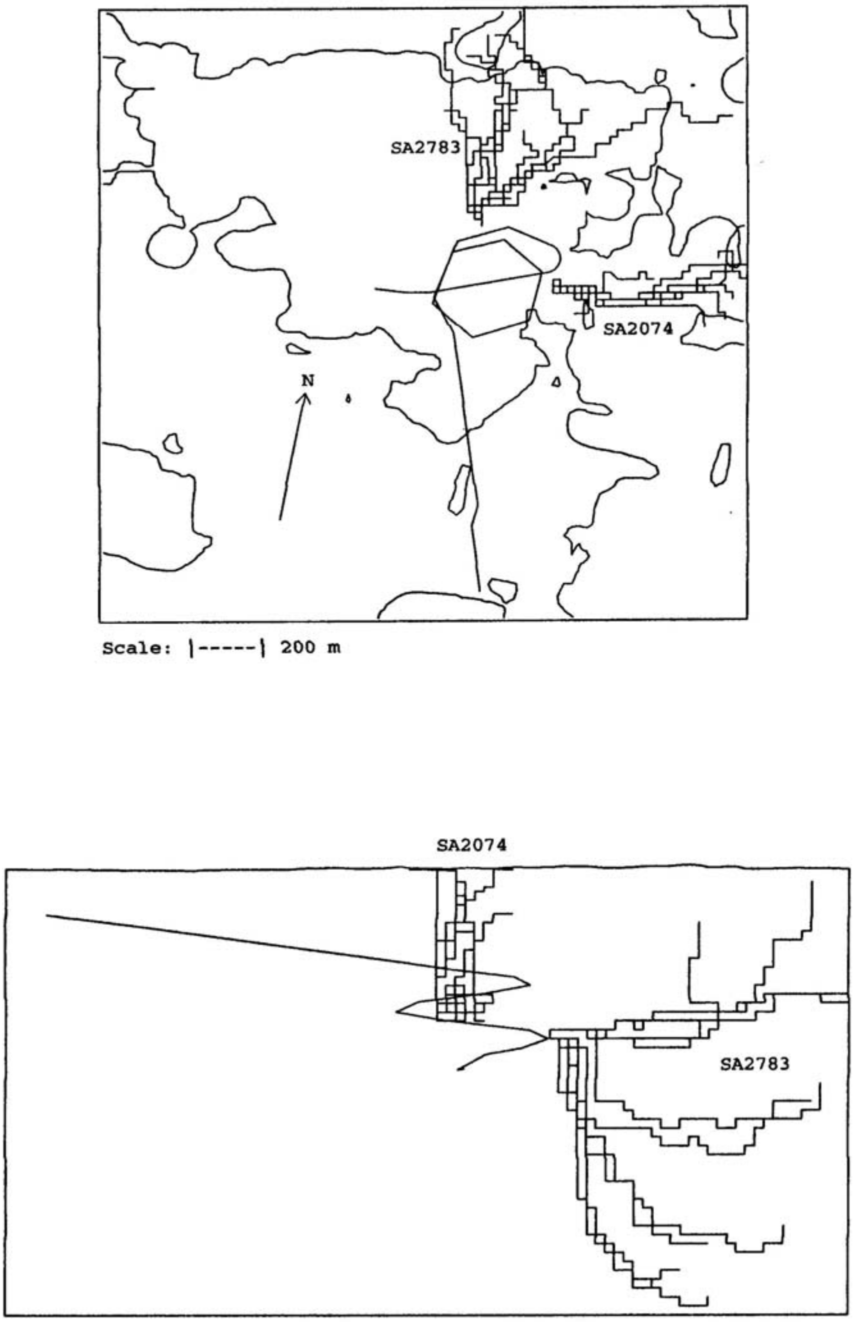


Figure 5-59. *Flow paths for water at control points SA2074 and SA2783. Horizontal view (top) and view from east (bottom). Tunnel front at 3 600 metres (Model 2). SKB/CFE (Svensson et al., 2002).*

Figures 5-60 to *5-65* show selected results of the modelled salinity and mixing proportions. The following conclusions were drawn:

- The main uncertainty about the four end member groundwater types concerned the boundary conditions (*Note that initial conditions were generated from a regional* *model based on Svensson (1997a)) in the present study. It was assumed that the same boundary conditions applied to all four vertical boundaries; this can be questioned.*)

- The hydrogeochemical data pointed to some shortcomings in the hydrological model. Field data indicated that Glacial Water had been stored for 12 000 years at a depth of a few hundred metres below Äspö. The method to generate the porosity field used in the study had the potential to store water for long time periods *(Svensson, 2001),* but it was considered that more work is needed before any firm claims can be made. Also, the kinematic porosity ought to be better founded on field data, than was possible in the study.

- Some detailed comments were:

    - The atmospheric pressure in the tunnel generated high pressure gradients close to the tunnel which resulted in an inflow of water. The low pressure around the tunnel was reflected at ground level. However, on the regional scale the Äspö HRL perhaps should be best considered as a 'point sink' that draws water from all directions.

    - Starting with water from the upper bedrock, the model showed that the Meteoric Water from Äspö (assumed to be 50 mm net recharge per annum) was not enough to explain the fraction of Meteoric Water inflowing to the tunnel. Possibly, Meteoric Water from the Laxemar area has provided a substantial part.

    - It was considered that the horizontal flow towards the tunnel followed the selective withdrawal principle, meaning that water from a certain density interval was mainly contributing to the inflow. This suggestion was given in *Svensson (1997a)* where the process is described and illustrated. The withdrawn water is replaced with water from above. This led to the expectation that the Glacial Water in the domain should steadily be replaced by Meteoric and Baltic waters. The decrease in Glacial Water was reflected both in the measured data and in the simulations.

    - Water with higher salinity than found at the level of the Äspö HRL under natural conditions was detected in the central part of the tunnel spiral. This was considered an indication of water transport from below the tunnel level, resulting in an upconing of saline water at the centre of Äspö HRL. It is interesting to note that the simulated maximum salinity continued to rise also after tunnel completion, a duration of 3.7 years (*Fig. 5-60*). Hence the salinity field was not in a steady state at 1997-01-01, which was the latest date the simulation was carried out to. As the transient salinity field affected the flow and pressure distributions, it was an indication that steady state site scale models can be questioned.

    - The transport time from the Baltic down to the tunnel was in range of a month (see Figure 5-64), which indicated the need for an intensive hydrogeochemical sampling programme near the tunnel face during excavation, when the tunnel was near ground surface.

All results presented, however, gave a plausible and consistent description of the evolution of the groundwater chemistry. Simulated salinity trends were largely in agreement with field data, with the exception of a slight decrease with time at the 2800 m tunnel coordinate (Fig. 5-60).

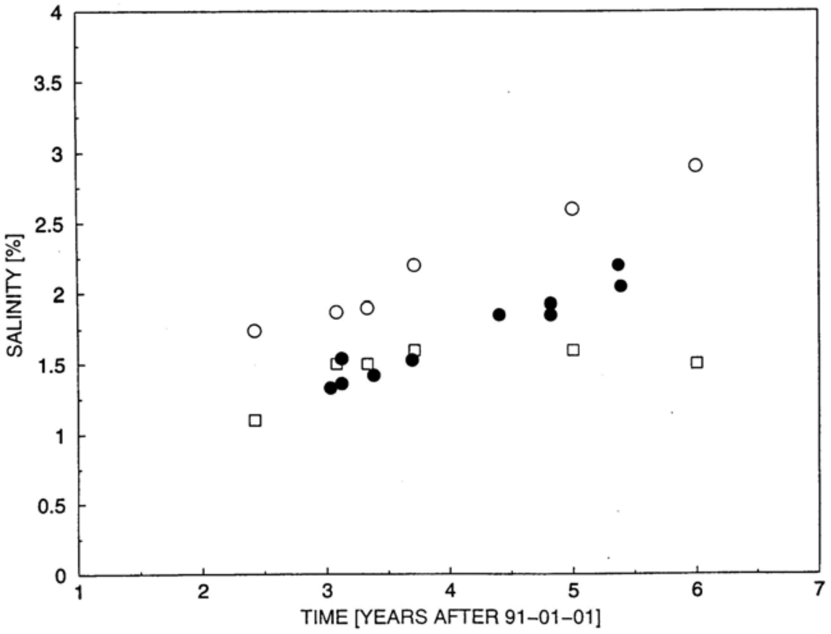


Figure 5-60. *The up-coning process where salinity is plotted as a function of time at a depth of 370 metres (Svensson et al., 2002).*

- ● *Field data (Control Points SA2783 and SA2880)*
- ○ *Simulated maximum salinity.*
- ☐ *Simulated salinity at tunnel coordinate 2 800 metres.*

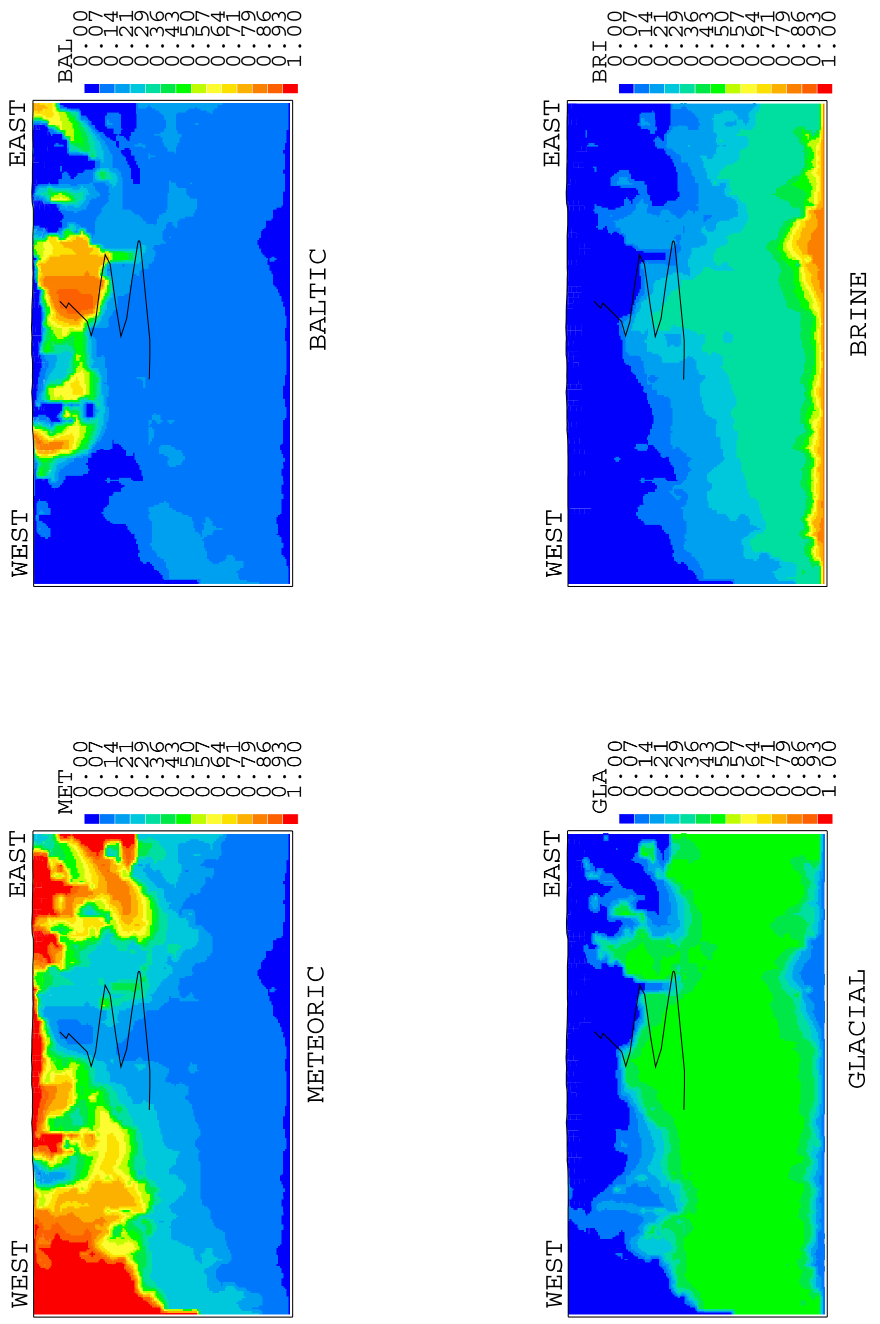


Figure 5-61. *Vertical sections in an E-W direction through the centre of the spiral part of the tunnel, showing the simulated distributions of various water types. Tunnel front position: 3170 metres. Model 2. (Svensson et al., 2002).*

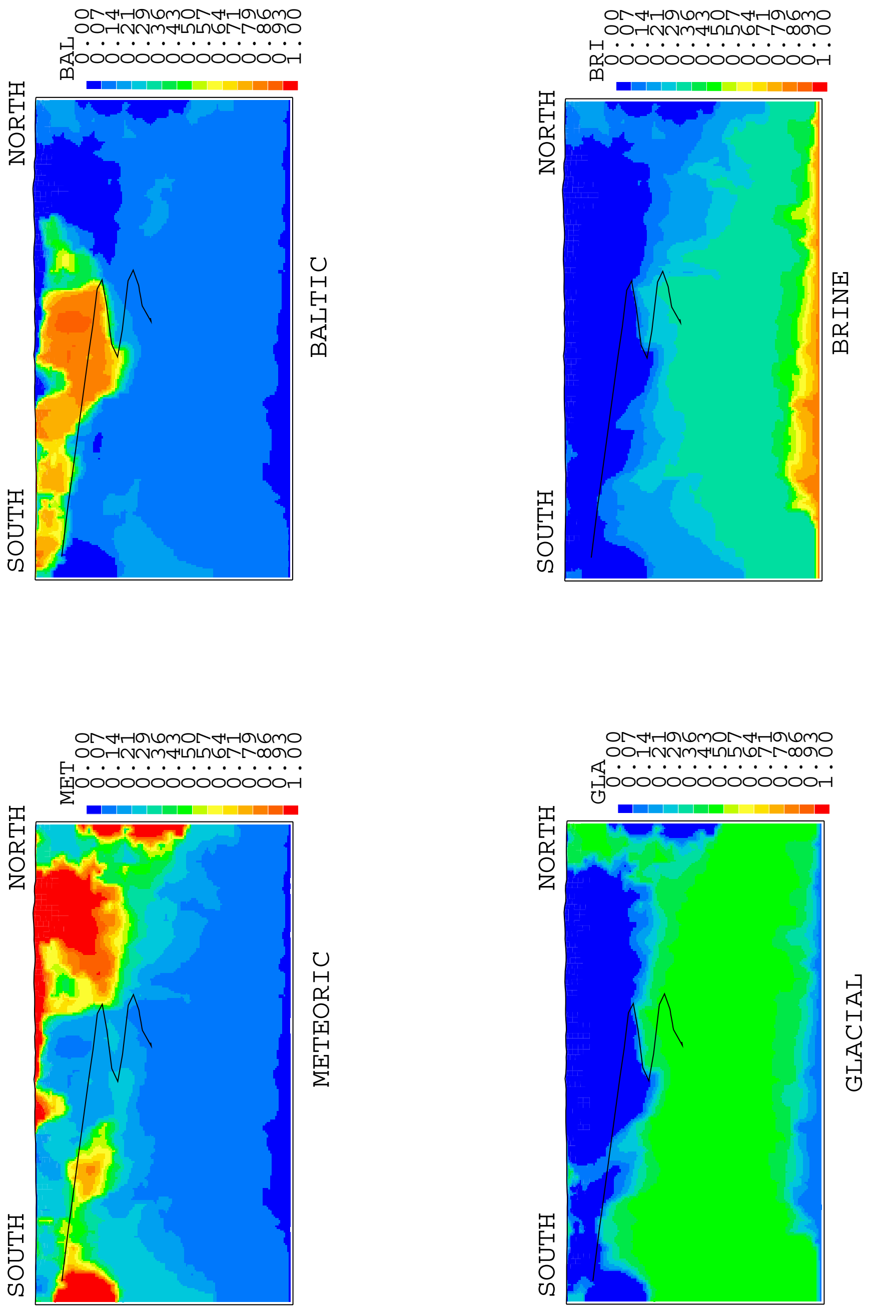


Figure 5-62. *Vertical sections in a N-S direction through the centre of the spiral part of the tunnel, showing the simulated distributions of various water types. Tunnel front position: 3170 metres. Model 2. (Svensson et al., 2002).*

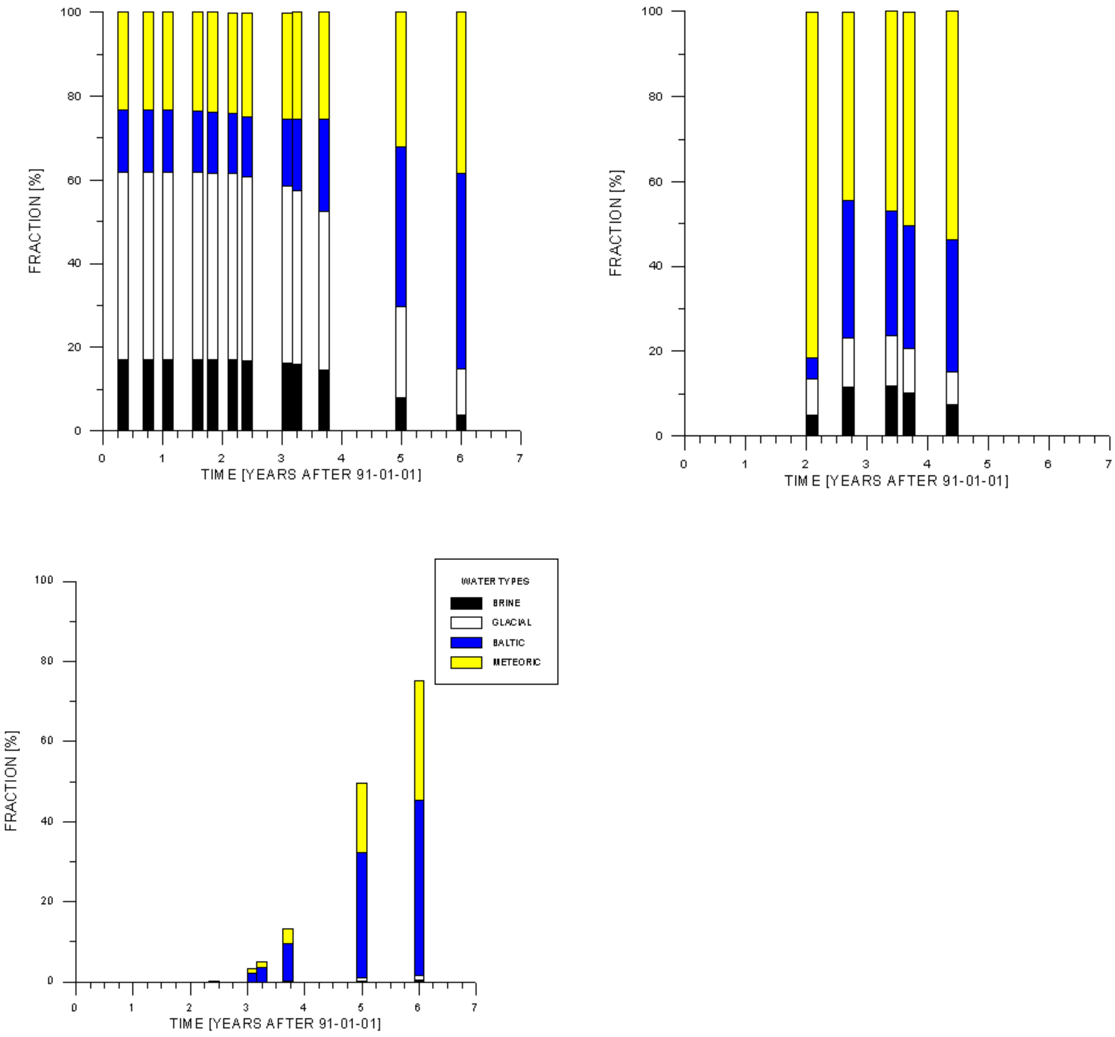


Figure 5-63. *Water composition at Control Point SA2074 as a function of time. Measured (top right) and simulated (top left) groundwater mixing proportions and fraction coming from the domain boundaries. Time when tunnel passed the control point: 2.09 years. Model 2. (Svensson et al., 2002).*

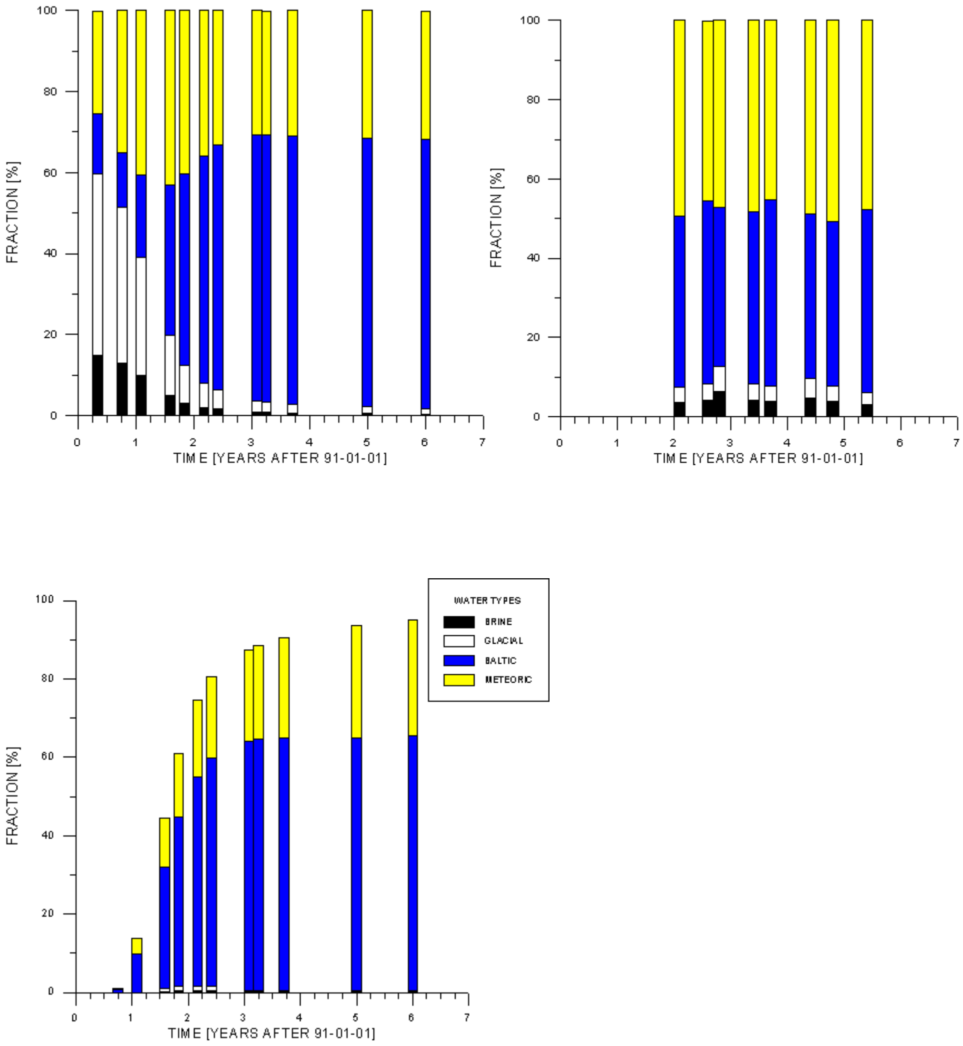


Figure 5-64. *Water composition at Control Point SA0813 as a function of time. Measured (top right) and simulated (top left) groundwater mixing proportions and fraction coming from the domain boundaries. Time when tunnel passed the control point: 0.58 years. Model 2. (Svensson et al., 2002).*

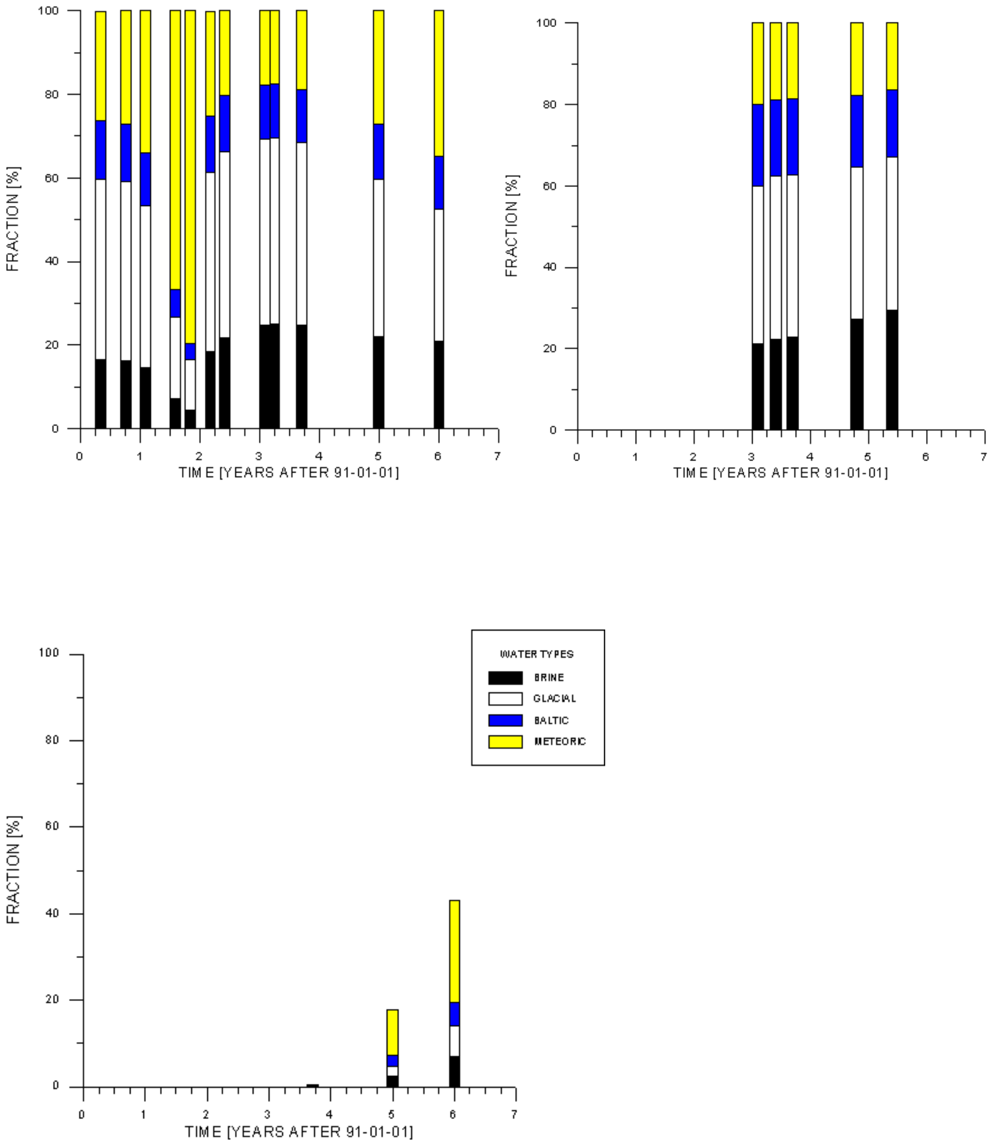


Figure 5-65. Water composition at Control Point SA2783 as a function of time. Measured (top right) and simulated (top left) groundwater mixing proportions and fraction coming from the domain boundaries. Time when tunnel passed the control point: 3.03 years. Model 2. (Svensson et al., 2002).

5.4.11 Summary and discussion

The modelled areas were approximately similar for all modelling groups (2 x 2 x 1 km^3). Four groups constructed a fully 3D model including the deterministically defined Hydraulic Conductor Domains (HCDs) and Hydraulic Rock Domains (HRDs). The remaining five groups modelled only the HCDs, referred to as a not fully "3D" model in the text, which influenced the parameters assigned to the HCDs when tested by calibration, and limited to some extent the use of the collected borehole information. Furthermore, it also limited the analysis of the possible pathways to control points. However all models showed the piezometric levels that were comparable to the measured ones, but a rather large spread of final (calibrated) parameter values for the HCDs and HRDs for the different groups was noticeable, probably to some extent dependent on a 3D or only a HCD modelling approach.

Modelling of groundwater flow into the tunnel can be made in two ways; a) distributing the measured flow rates as prescribed fluxes along the tunnel as a time dependent series, or b) assuming atmospheric pressure in the tunnel and adding a skin (hydraulic resistance) around the tunnel to get the measured flows. The modelling groups used one or the other of these methods and adopted different ways of carrying out the transient simulations; some made true transient simulations whilst others made step-wise stationary solutions of the pressure and flow field for defined tunnel face positions.

All available data were not used to test and calibrate the models. Further more, only limited sensitivity studies were made; this was due to the limited resources (money and time) given the large amount of data that were supplied.

All groups identified a number of different uncertainties in the final models presented and these uncertainties differed considerably between the groups. Partly it reflected the modelling approaches, but equally it reflected the difficulty of how to handle such a large quantity of data and find a structured, step-wise approach to build and test models using these data. However, all groups had one thing in common, all identified the problem of how to assess reasonable initial conditions based on a rather sparsely distributed data set, except for around the Äspö tunnel. Another problem was that the transient simulations indicated that after some years, groundwater from the vertical boundaries entered into the tunnel. The size of the modelled areas (about 2 x 2 x 1 km^3) was not large enough to avoid that effect.

The use of groundwater mixing proportions, and sometimes the chemical constituents, where considered to have improved confidence in the models constructed. Furthermore, hydrogeochemistry made it possible to assess the transport properties of the rock.

5.5 Estimating the influence of chemical reactions

5.5.1 General

Using the M3 modelling approach the degree of groundwater mixing could be estimated and the contribution of chemical reactions during groundwater mixing indicated (see section 3.5). However, the potential role of water-rock interaction still needed to be further quantified. As part of Task 5, each modelling group was therefore requested to indicate which water-rock reactions they considered as being of major importance, how they intended to model these reactions (thermodynamics vs kinetics), and how they expected to integrate these data in their respective hydrodynamic models. A list of six major reactions was identified by SKB for consideration; these are listed and described in sub-section 3.5.2. Table 4.2 indicates the six groups which have considered the influence of chemical reactions and summarises the reactions of importance addressed by each group.

5.5.2 ANDRA/ITASCA

The ANDRA/ITASCA group applied a fully coupled reactive transport model (3FLO) to part of the model domain. The geochemical modelling approach assumed thermodynamic equilibrium; reaction kinetics were considered either very fast or very slow with respect to the groundwater residence times and were therefore not addressed. Chemical species were preferred to the M3 end member mixing ratios; the principle components (i.e. initial conditions) selected were Na^+, K^+, Ca^{2+}, Mg^{2+}, CO_3^{2-}, Cl^- and SO_4^{2-}. The major reaction addressed was that of calcite dissolution/precipitation (see section 3.5.2); this was extended to include magnesium carbonates and gypsum even though, as pointed out by the authors, the inclusion of magnesium carbonate was unrealistic in the context of the Äspö system. Using the CHEMVAL database all relevant soluble chemical complexes to this calculation where included.

The ANDRA/ITASCA fully coupled modelled simulations can be summarised as follows:

- Coupled modelling was used to simulate the impact of tunnel construction over a period of 100 days.
- Simulations indicated that variable water salinity influences the aqueous solution ionic strength and consequently the 'apparent' chemical reaction constants.
- Reactive transport results showed that even in zones where geochemistry was considered as simple and of little importance (e.g. in the absence of significant redox or surface reactions), transport of chemical species might in fact be affected by mineral precipitation/dissolution, therefore constraining the hydrodynamic modelling.

5.5.3 BMWi/BGR

The approach of BMWi/BGR was based on the premise that water-rock reactions reflecting deviations from an ideal mixing model could be identified by applying a geochemical thermodynamic equilibrium model. The program used was PHREEQC (Version 2) which handles speciation, batch reaction and inverse geochemical calculations, and provides information on which processes dominate and to what extent, and which constituents and pure phases participate in the reactions. The input data consisted of measured time-series groundwater chemistry and the most important chemical species used were Na^+, Cl^-, δ^2H and $\delta^{18}O$ (conservative species) and K^+,Ca^{2+}, Mg^{2+}, HCO_3, CO_3^{2-}, and SO_4^{2-} (non-conservative or reactive species).

Using the same end members as derived from the M3 calculations (i.e. Baltic Sea, Glacial, Meteoric and Äspö Brine), the first step was to calculate the proportions of the different groundwater end members for each groundwater sample. This was carried out using chloride, sodium and ^{18}O as conservative tracers; the resulting mixing proportions were then used to determine the non-conservative or reactive elements. Plots comparing calculated with measured values showed a clear deviation from the ideal mixing line for the non-conservative elements, much less so for the conservative tracers. The general distribution of the plotted data was similar to that calculated by the M3 method.

Potential chemical reactions selected to explain the observed deviations for the reactive elements included:

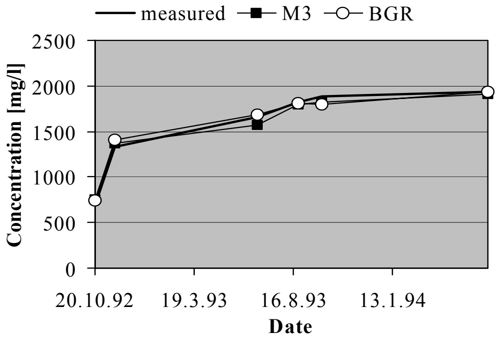
- Dissolution/precipitation of carbonate (gain of HCO_3; loss of Ca^{2+})
- Dissolution of gypsum (gain of SO_4^{2-})
- Dissolution of dolomite (gain of Mg^{2+})
- Cation exchange (loss of K^+; gain of Na^+ and Mg^{2+})
- Organic decomposition (gain of HCO_3)
- Organic redox reactions (gain of HCO_3)
- Oxidation of pyrite/organic matter (gain of SO_4^{2-})
- Degassing of CO_2 (loss of Ca^{2+}; loss of HCO_3)

The influence of chemical reactions was modelled using PHREEQC and resulted in a revised set of groundwater mixing ratios that corresponded much closer to the measured values; this supported the importance of chemical reactions in the sampled groundwaters. *Figure 5-66* shows the results from one control point comparing the recalculated simulations using chemical reactions with the measured values. (*Summary Report Author's Note: The calculated M3 values also are included, although since these calculated data relate to the site as a whole and not to one specific control point, a direct comparison is not valid*).

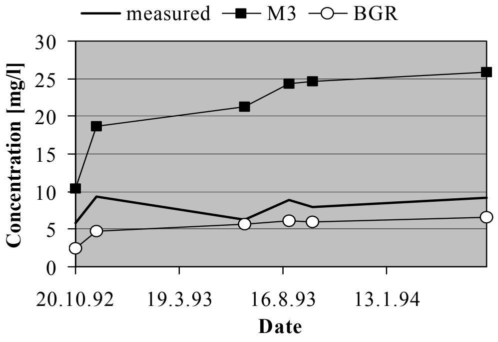
Additionally, using PHREEQC, BMWi/BGR conducted some equilibrium batch reaction calculations on two selected boreholes with suitable time-series data collected during tunnel construction. The exercise was based on the assumption that chemical reactions controlling the ion content can be identified by knowing the saturation indices of different minerals in the water samples measured at different times. As the saturation state of some specific mineral phases change significantly with time, then these minerals probably are involved in the chemical processes. An increase or decrease in the saturation state of these minerals during tunnel construction therefore may shed some light on the dynamic mixing of different groundwater types, for example due to drawdown or upconing processes. However, this approach gives no clear evidence of the actual flow or progress of theses reactions.

The selected minerals were chosen on the basis of mapped fracture filling minerals in the laboratory tunnel. Based on the batch calculations, which were applied to the whole computational domain of the fracture network grid used in the hydrodynamic modelling, a change in calcite and dolomite towards subsaturation was observed with time. As meteoric water shows a clear subsaturation concerning calcite and gypsum, and the penetration depth of meteoric water increases with time, the general evolution at the site indicates a move towards a higher subsaturation of these minerals. Consequently the calculations implied active mineral dissolution with time. However, the saturation index of $CO_2(g)$ also showed a clear decrease which may be due to a degassing of $CO_2(g)$ owing to a decrease in pressure during the tunnel construction.

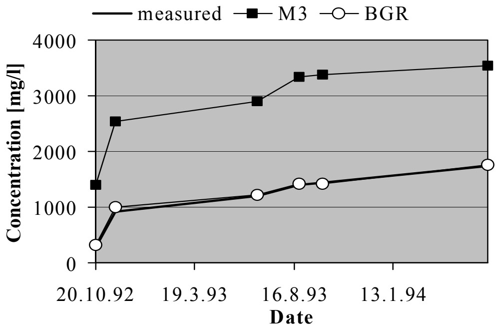
Na^+ in SA1696B:



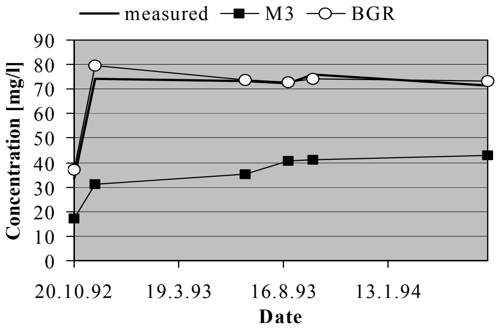
K^+ in SA1696B:



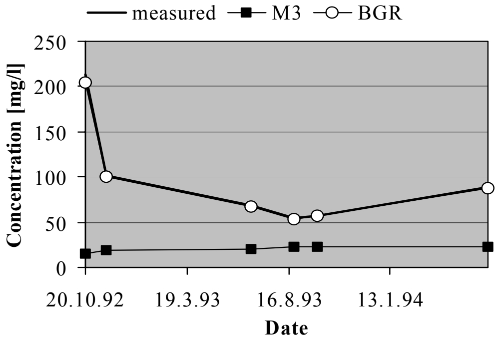
Ca^{2+} in SA1696B:



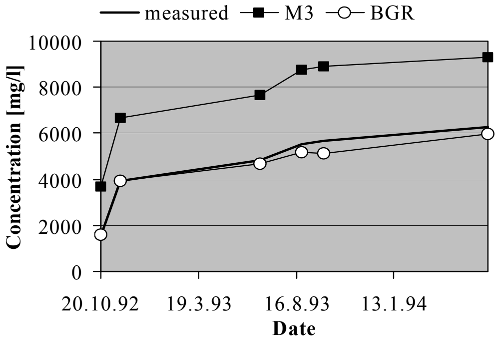
Mg^{2+} in SA1696B:



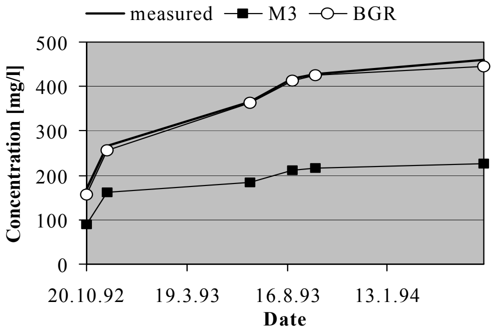
HCO_3^- in SA1696B:



Cl^- in SA1696B:



SO_4^{2-} in SA1696B:



^{18}O in SA1696B:

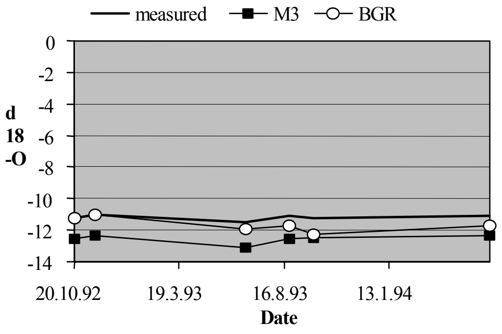


Figure 5-66. *Measured element concentrations in borehole SA1696B compared to a mixing-equilibration approach (Liedtke and Klennert, 2002).*

5.5.4 CRIEPI

The approach of CRIEPI shared certain similarities with that of BMWi/BGR. The initial compositions of the four recommended groundwater end members were first defined, based on the measured chemistry. The chemical species of the mixed waters (i.e. sampled at the selected control points) were then calculated from the mixing proportions as predicted from the M3 results. This exercise was repeated using alternative groundwater mixing ratios (using Cl and ^{18}O as conservative species) generated by the FEGM/FERM code for groundwater flow and solute transport. Finally, these mixed water proportions were modelled using the geochemical equilibrium HARPHRQ code (i.e. based on PHREEQE and using the HATCHES database) to identify which major geochemical reactions had contributed to the calculated chemistry. Cation exchange reactions were also considered assuming 20% clay and that clay minerals within 0.1mm in depth from the fracture surface participate.

The most important reactions considered in the modelling were:

- HCO_3 production from decomposition of organic material
- Near-surface (i.e. meteoric water) consumption of dissolved oxygen by pyrite oxidation
- Dissolution and precipitation of calcite
- Cation-exchange between Ca and Na by clay minerals
- Oxidation/reduction between HS^- and SO_4^{2-}

The modelling results of the chemical reactions using the FEGM/FERM-derived groundwater mixing proportions are given in *Figure 5-67*. The results showed that the decomposition of organic material appears to control the concentration of HCO_3^- in the majority of cases and cation-exchange reactions were significant. By taking both these reactions into consideration (in particular cation-exchange) resulted in a closer agreement with the measured values. The effect of the HS^- and SO_4^{2-} on groundwater redox conditions was not considered significant.

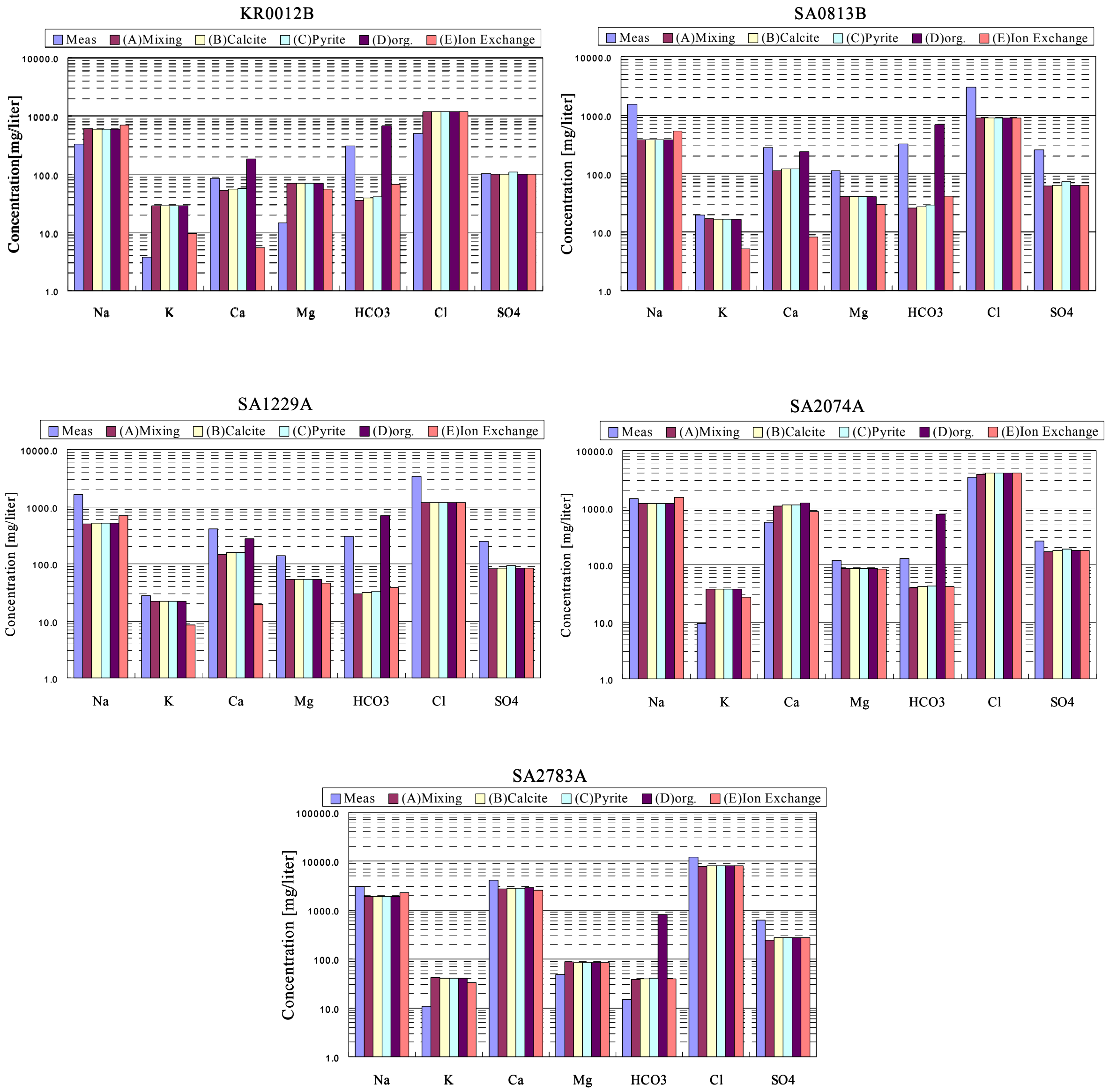


Figure 5-67. *Influence of the five main chemical reactions on chemical concentrations from five control points; based on the FEGM/FERM code. (Hasegawa et al. (2002).*

5.5.5 ENRESA/UDC

ENRESA/UDC did not hydrogeochemically model the influence of chemical reactions during groundwater mixing as part of the Task 5 exercise. However, outside the framework of the project they carried out numerical simulations on the Redox Zone, which intersects the access tunnel at 70 m depth (*Banwart et al., 1999*). The simulations were carried out using the CORE^{2D} finite element code which solves groundwater flow, heat transport and multi-component reactive solute transport under variably saturated conditions (*Molinero et al., 2002*; Appendix 5). This coupled groundwater flow and reactive solute transport model is used to perform reactive transport simulations accounting for aqueous complexation, acid base reactions, redox processes, cation exchange and mineral dissolution/precipitation. The model accounts for more than 60 reactions, including aqueous complexation, acid-base reactions, gas dissolution and redox processes, as well as reactions including mineral dissolution/precipitation and cation exchange. The model reproduces the measured hydrogeological response, as well as the observed concentrations of most dissolved species both before and after tunnel construction.

Figure 5-68 A shows a comparison between measured and computed concentrations for undisturbed (natural) conditions at the future tunnel location. In general, a very good agreement between computed and measured concentrations (at a depth of 70 m) was achieved. As expected, the most important discrepancies were found for dissolved sulphates, bicarbonates and iron which can be affected by microbial processes not considered in the numerical model. *Figure 5-68 B* shows the comparison between measured and computed chloride concentrations during the Redox Zone Experiment (after the tunnel intersected the fracture zone).

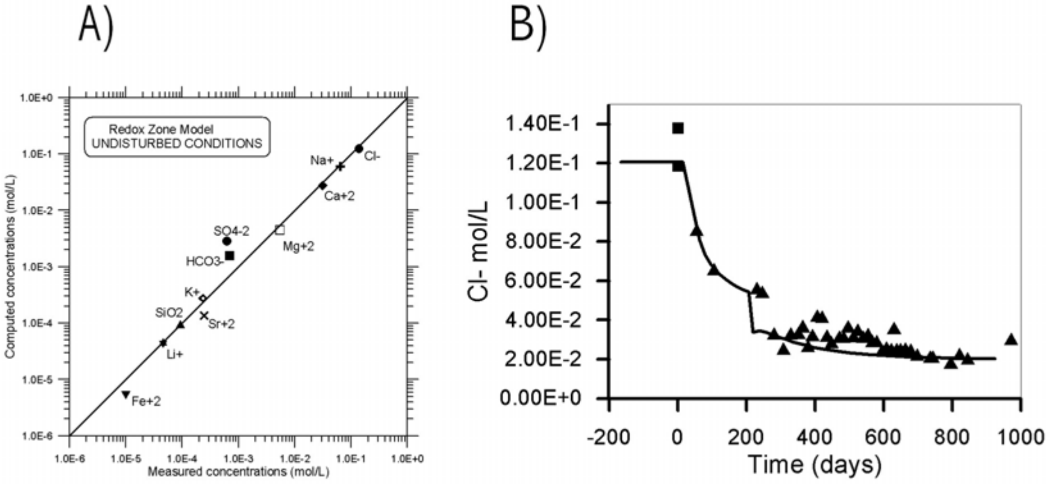


Figure 5-68. *Comparison between measured and computed concentrations for undisturbed conditions at the tunnel location (70 m deep). (Molinero et al., 2002).*

Generally this model was able to reproduce the observed behaviour of most dissolved species. However, some discrepancies were found for dissolved bicarbonates and sulphates and, as mentioned, a possible explanation for these discrepancies is the occurrence of microbially catalysed processes. Since microbially-mediated processes have been documented at Äspö, these processes were incorporated into the ENRESA/UDC reactive transport model, in effect producing a hydrobiogeochemical model (BIO-CORE). *Figure 5-69* shows the computed concentration evolution of bicarbonate and sulphate as well as the comparison with measured data (at the tunnel depth). This figure also shows the numerical results computed without including microbially mediated iron reduction-DOC oxidation processes (the hydrogeochemical base model). It is worth noting that including these microbially catalysed processes, the numerical model (the hydrobiogeochemical model) was able to reproduce the measured behaviour of bicarbonates and sulphates during the time of the Redox Zone

Experiment. This constituted quantitative evidence of sulphur organic matter oxidation being the source of bicarbonate and sulphur.

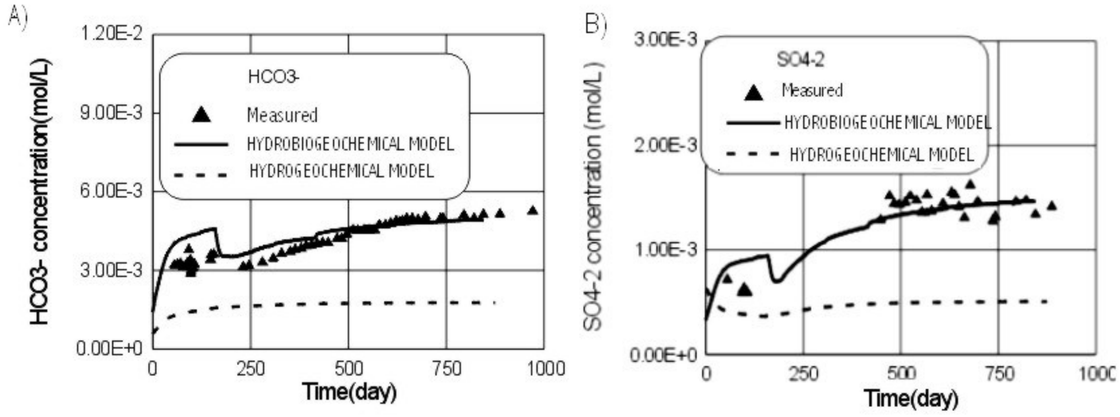


Figure 5-69. *Comparison between measurements (symbols), hydrobiogeochemical model results (solid line) and hydrogeochemical model results (dashed line) for: A) time evolution of dissolved bicarbonates and, B) time evolution of dissolved sulphates. (Molinero et al., 2002)*

ENRESA/UDC pointed out the importance of such hydrobiogeochemical modelling since microbially mediated processes can be of great relevance in performance assessment exercises of deep geological repositories hosted in crystalline bedrock. (*Summary Report Author's Note: The Redox zone study was restricted only to shallow depths around 70 m and is not, therefore, typical of repository depths*).

5.5.6 JNC/Golder

The hydrochemical modelling approach of JNC/Golder, detailed below in sub-section 5.7.2, was based on a PCA analysis and, in common with the M3 approach, provided only a qualitative indication of which chemical reactions were occurring and their relative importance. No effort was made to hydrogeochemically model the influence and importance of these reactions.

5.5.7 Posiva/VTT

The hydrogeochemical approach of Posiva, detailed below in sub-section 5.7.3, was based on an inverse-modelling approach which combined speciation modelling and mole balance modelling. Providing constraints on the modelling included detailed mineralogy, reactions expected to dominate in the groundwater system and groundwater isotopic data. The computations were handled by the PHREEQC (Version 2) program, similar to that used by the BMWi/BGR group. Understanding the groundwater reaction geochemistry therefore formed a central part of the study.

5.5.8 SKB/CFE

The hydrgeochemical modelling approach of SKB/CFE, detailed above in Section 5.2, was based on M3 calculations and provides only a qualitative indication of which chemical reactions are occurring and their relative importance. The reactions SKB/CFE identified as being potentially important are listed in sub-section 3.5.2. No effort was made to hydrogeochemically model the influence and importance of these reactions.

5.6 Alternative hydrogeochemical approaches

5.6.1 General

The groundwater mixing proportions based on M3 calculations were used by all modelling teams in the hydrodynamic simulation exercises thus providing common ground and facilitating comparison and integration. The M3 method therefore played an important central role in the successful execution of Task 5. However, the M3 method is not the only approach available to derive reference end member groundwaters and to calculate mixing ratios. Posiva/VTT developed a method some time ago that has been applied successfully to their hydrogeochemical site characterisation evaluation programme (e.g. *Pitkänen et al., 1996, 1999*). This alternative approach was also applied to the Task 5 data and is reported in *Luukkonen and Kattilakoski (2001).* Moreover, as a direct spin-off from the Task 5 modelling, was the development of a method by the JNC/Golder group and reported in *Dershowitz et al. (2001)*. This development was driven by domestic Japanese requirements, namely fresh water systems where water-rock interactions are more prevalent. Details of these alternative approaches are described briefly below.

5.6.2 JNC/Golder

The JNC/Golder modelling approach primarily addressed the hydrogeochemical uncertainties in the chemistry and mixing proportions of different end members as derived by the M3 calculations. The statistical method adopted was essentially based on 'a chemometric algorithm which made no initial assumptions about the nature of the end members present, and which considered all the contributions to chemical variability in the groundwaters' *(Dershowitz et al., 2001).* The approach is schematically shown in *Figures 5-70* and *5-71*. In *Figure 5-70* matrix A is known and matrices B and C require to be calculated; *Figure 5-71* illustrates the four-stage process used to determine B and C, i.e. the mixing proportions and estimated end member compositions. With respect to the new chemical components obtained from the model calculations:

- They were not principal components, but were derived from principal components,
- They were not end members, but could be considered analogous to the end members identified from the M3 modelling, and
- They should show some similarity in composition with the M3-derived components

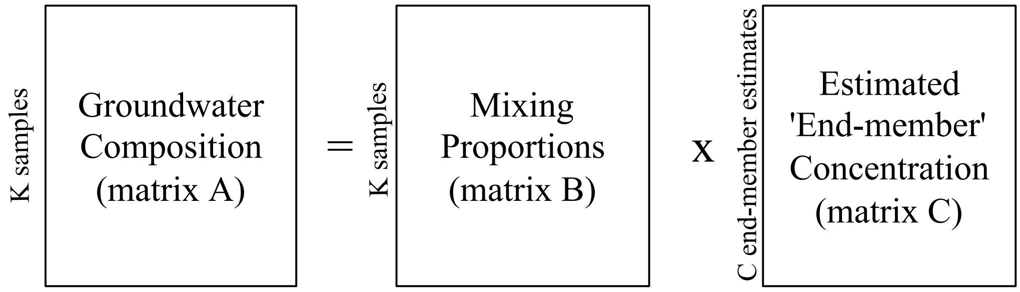


__Figure 5-70.__ Relationships between matrices used in the revised modelling (Dershowitz et al., 2002).

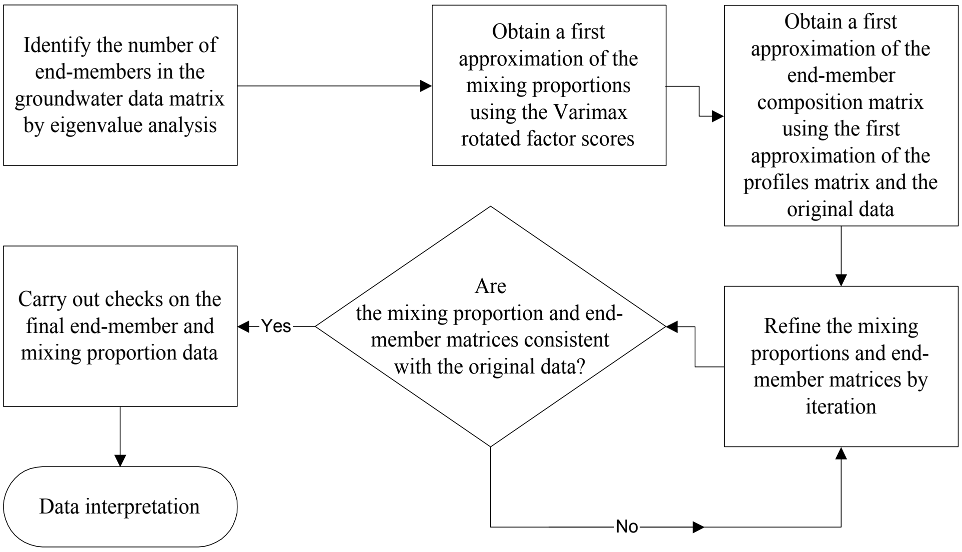


__Figure 5-71.__ Summary of the procedure adopted in the revised modelling (Dershowitz et al., 2002).

The modelling results were then compared to the M3 calculations by expressing the new mixing proportions in terms of proportions of the original M3 end members. Several different modelling approaches were evaluated and the same data input to produce the M3 calculations was used in some of the models to facilitate comparison. For example, the comparison between proportions of end members calculated by M3 and JNC/Golder is shown in *Figure 5-72*. The plot shows a general positive correlation between the two approaches, particularly with respect to Äspö Brine but less so for Baltic Sea and Meteoric waters where JNC/Golder calculated higher proportions of Baltic Sea at shallower depths (<400 m) and lower proportions of Meteoric Water at greater depths (>400 m). The calculations also predicted negative proportions of Meteoric Water for some samples which, although appearing unrealistic, actually correspond to a large negative deviation between theoretical and measured chloride concentrations calculated by M3.

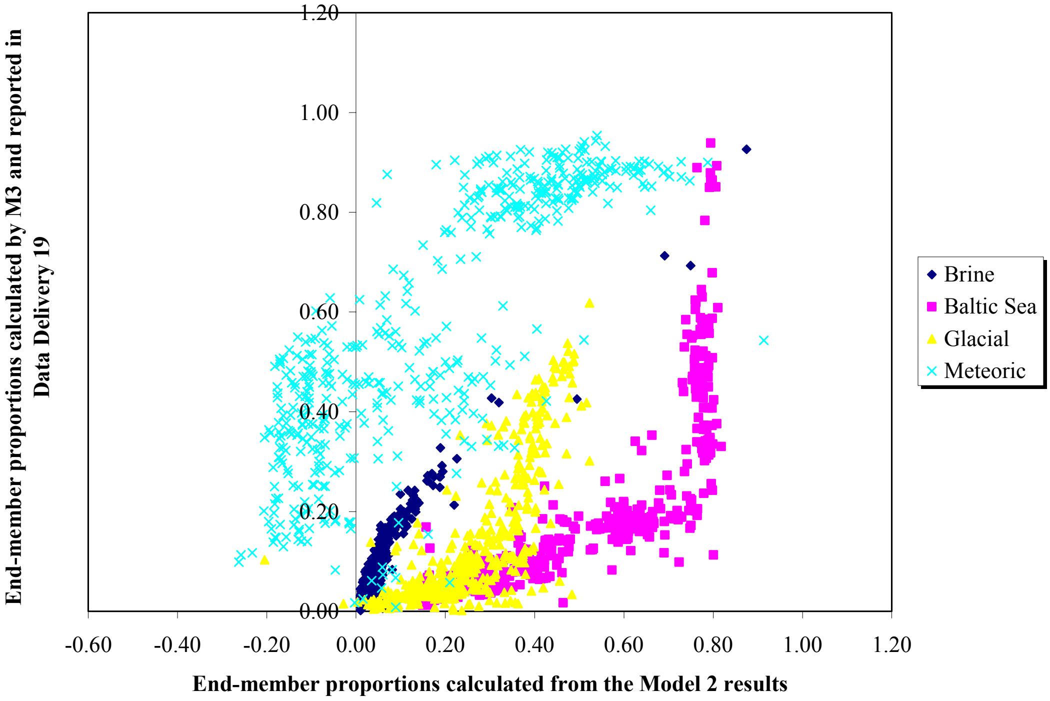


Figure 5-72. *Comparisons between proportions of end members calculated by M3 and released by SKB in Data Delivery 19, and proportions of the same end members calculated using the revised Model 2. (Dershowitz et al., 2002).*

The main conclusions from the JNC/Golder modelling after *Dershowitz et al. (2002)* were:

- even though the results were largely consistent with the M3 calculations, the JNC/Golder approach was considered more applicable since it considered all groundwater chemical variability; seven principle components were employed
- the method distinguished clearly between mixing and water-rock reaction processes
- stable isotope and hydrogen isotope data were necessary to ensure an internally consistent model
- tritium had a relatively large effect on the calculations because of its short half-life; variations in tritium could be explained by decay rather than by groundwater mixing
- inclusion or exclusion of extreme groundwater constituents or groundwater types had a significant effect on predictions
- the proportions of Äspö Brine in any groundwater were probably reliable
- Some of the M3-derived end members might not be present at Äspö; Meteoric Water did not always seem to be present at intermediate depths

5.6.3 Posiva/VTT

The Posiva/VTT modelling approach reported in *Luukkonen and Kattilakoski (2001)* was based on inverse modelling that described the chemical evolution of groundwater by giving exact estimates of the mixing and geochemical reactions among known initial groundwater compositions needed for reaching a known final groundwater composition. The steps involved in this process, which assumed steady-state chemical reactions, were extended to identifying reference waters and ultimately determining their mixing proportions in each groundwater sample. The modelling was carried out using PHREEQC (Version 2) (*Parkhurst and Appelo, 1999*); one advantage of this code was its advanced handling of uncertainties.

Since different groundwater end members were used in the Posiva/VTT approach, plus different criteria employed in calculating the mixing ratios, this approach could not be compared directly with the M3 calculations and therefore formed a separate study within Task 5.

The initial task was to establish the number and type of reference waters or end members. A total of seven reference groundwaters were identified which correspond to four, hydrogeochemically significant stages: Present, Litorina, Glacial and Preglacial. The reference groundwaters selected were Meteoric Water, Seawater, Postglacial Water (seawater that had infiltrated bottom sea sediments), Litorina Sea Water (7 500-7 000 BP), Glacial Melt Water (Pleistocene), Preglacial Altered Water (deduced from Quaternary history) and Saline Water (most saline sample at Äspö).

Using these end members, the next task was to carry out the stepwise calculations. Diagrammatically these calculations are shown in *Figure 5-73* were REF A to REF E represent the five reference waters selected together with seven groundwater samples (S1-S7). The choice of the steady-state steps was based on identification of the geochemical affinities for each groundwater sample, and finding a suitable water assemblage for each of these seven samples (i.e. solid tie-lines in the figure). The calculation approach can be summarised as follows:

- The calculations were carried out in steps, assuming steady-state chemical reactions
- The calculations were based on the assumption that Cl and ^{18}O behaved conservatively
- All other chemical values used in the calculations were subject to mole transfers, i.e. they were involved in dissolution/precipitation to/from reacting phases to satisfy the calculation constraints
- The directions of dissolution/precipitation reactions moved towards achieving steady-state conditions
- A previously successful step (assuming steady-state) lead to the next step
- These steps ultimately extended to the reference waters, and then to the mixing fractions
- In general, the more steps that were close to the reference water types, the more realistic the results, i.e. pure mixings between two reference waters were better avoided.

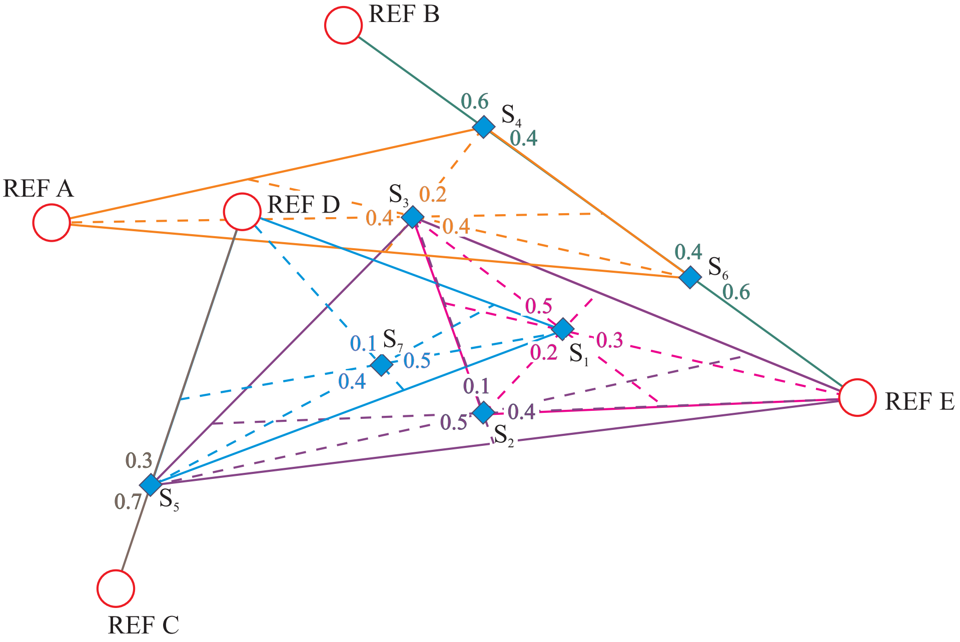


Figure 5-73. *Diagrammatic presentation of the stepwise calculation of reference water-type mixing fractions in given water samples. Samples used as initial waters for a certain final water are linked by solid tie-lines. Broken lines illustrate the rough euclidean distance of initial waters from a final water sample. Solid and broken lines, and given mixing fractions related to the same final water sample, are given the same colour. (Luukkonen and Kattilakoski, 2002).*

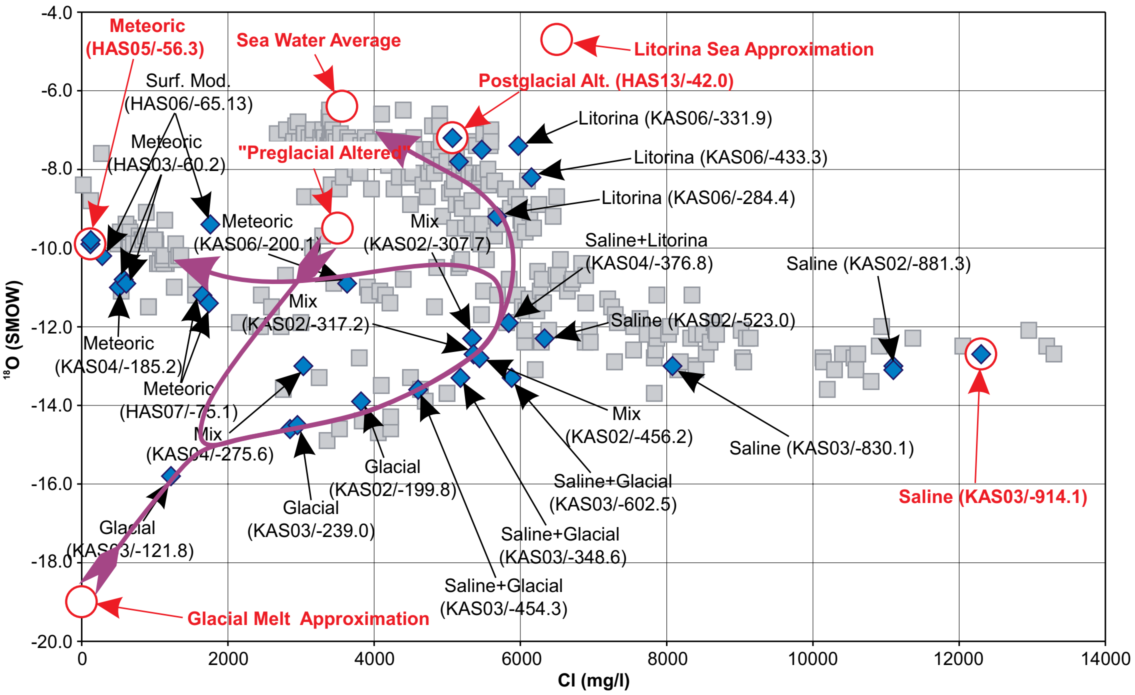


Figure 5-74. *Schematic overview of the mixing evolution in shallow depth groundwaters at Äspö. Violet arrows show assumed evolution trends below sea and land areas. (Luukkonen and Kattilakoski, 2002).*

Applied to shallow, undisturbed conditions at Äspö, *Figure 5-74* gives a schematic overview of the groundwater mixing evolution based on the inverse modelling approach. *Luukkonen and Kattilakoski (2001)* applied this method to the disturbed tunnel conditions, but again no direct comparison could be made with M3 because of the different end members selected and also the fact that the inverse model approach, unlike M3, is not mathematically based.

The general conclusions from the Posiva/VTT study were:

- Results showed three extensive sources of reference groundwaters that attempted to intrude into the Äspö site during open tunnel conditions.
- These reference groundwater types were Meteoric Water, fresh Baltic Seawater and Saline Water.
- Geochemical reactions related to these types were strong (Baltic), moderate (Meteoric) and weak (Saline).

5.6.4 Summary and discussion

JNC/Golder and Posiva/VTT carried out independent methods to calculate the mixing proportions of reference end member waters and the sampled groundwaters. These serve as alternative approaches to the M3 calculations in different respects. The JNC/Golder approach is, in common with M3, statistically based and shares many similarities, but goes one step further in that selection of the chemical components (partly analogous to the M3 end members but also containing components that represent other sources of variation, such as reactions) and mixing proportion calculations are based on all the chemical variability of the dataset. This ensures a more objective choice of 'end members' and, in turn, increases confidence in the quality of the calculated groundwater mixing proportions. In contrast, the Posiva/VTT approach is not mathematically-based but has the great advantage of integrating chemical reactions; an obvious disadvantage is the necessity of a substantial input of expert judgement.

These model developments are viewed as a very pleasing example of continued improvement in hydrogeochemical evaluation methodology that has been stimulated by the M3 modelling. M3, as with any modelling tool, has its weak points, the discussion of which lies outside the scope of this Summary Report (see Task 5 Review Report (*Bath and Jackson, 2002*) for detailed discussion), but it is a quick and convenient method to initially classify large hydrogeochemical data sets given the Äspö type hydrodynamic groundwater environment. As pointed out by JNC/Golder, however, it may not be so suitable for shallow, fresh-water environments characterised by reactions rather then mixing. The Posiva/VTT methodology has its place in the detailed hydrogeochemical understanding of the groundwater flow system, but it can be time-consuming and requires detailed knowledge of the system.

6 Summary and overall conclusions

Traditionally, with only some exceptions, modelling groups specialising in hydrogeology and hydrogeochemistry have tended to work in parallel rather in close collaboration. The Task 5 modelling exercise represented a coordinated attempt to bring together these two groups and to integrate closely hydrogeochemistry with hydrogeology in the light of future repository site characterisations and performance assessment requirements.

6.1 General Summary of the Task 5 Modelling Exercise

The principle aim of the Äspö Task 5 modelling exercise has been to compare and ultimately integrate hydrogeochemistry and hydrogeology using the input data from the pre-investigation and construction phases of the Äspö Hard Rock Laboratory (HRL). The main objectives were:

- to assess the consistency of groundwater-flow models and hydrogeochemical mixing-reaction models through integration and comparison of hydraulic and hydrogeochemical data obtained before and during tunnel construction, and
- to develop a procedure for integration of hydrological and hydrogeochemical information which could be used for disposal site assessments.

The rationale behind these modelling exercises is based on the following:

- groundwater flow and chemistry are important for the safety and performance assessment of a deep geological disposal of radioactive waste,
- if groundwater flow and chemistry are integrated properly, it should give better confidence in the description of present and future conditions at a potential repository candidate site, and
- the modelling approaches used in Task 5, if considered successful, could be used for any future repository site investigations and evolution, especially in a crystalline rock environment.

In order to facilitate comparison, a series of control points were identified along the tunnel. These locations mostly relate to the intersection of the tunnel with hydraulically active fracture zones and form part of the long-term monitoring programme where measurement of hydraulic parameters and hydrochemical sampling are routinely carried out. Based on these tunnel locations, a series of measures were identified to check the performance of the models. These performance measures are:

- the nature of the groundwater flow pattern through the bedrock to the tunnel control points
- the advective groundwater travel time distribution to the control points, and
- the nature of the groundwater chemical evolution to explain the results at each control point.

Two different modelling aims were specified: a) tunnel section 0-2900 m was chosen for model calibration and all pre-construction and construction data were made available, and b) tunnel section 2900-3600 m was chosen for model predictions where only the pre-investigation input data were made available; the objective was to predict the construction phase disturbance.

6.1.1 General issues

- Groundwater mixing ratio simulations based on M3 calculations provided a convenient means to integrate hydrogeochemistry and hydrogeology.
- The simulations showed that the results over the time period simulated (about 5 years) were sensitive to the boundary conditions of the 'regional model' with dimensions of approximately 2 x 2 x 1km (last figure is depth). Simulations indicated that the transport times from the vertical boundaries were possibly shorter than the simulation time, thus having a great impact on the simulated chemical composition of the inflowing water to the tunnel at the control points.
- The reliability of the given boundary conditions was an issue discussed at length, especially the western boundary, since it was mainly based on one deep borehole.
- Another issue addressed was whether the hydrogeochemical data could represent conditions in the entire rock mass or mainly the most conductive features, i.e. the issue of how to interpolate in a reasonable way to obtain initial and boundary conditions solely for the Hydraulic Conductor Domains (HCDs) and Hydraulic Rock Domains (HRDs).
- Below the Baltic sea the shortest transport times from the boundaries (sea bottom) was in the scale of approximately one month, indicating that the sampling programme carried out was inadequate to record the rapid dynamics of the system during tunnel construction.
- A full and direct comparison between modelling groups was not possible due to different levels of ambition, achievement, available time and resources and model development.

6.1.2 Groundwater mixing proportions

- Results showed M3 to be a satisfactory semi-quantitative tool to calculate mixing proportions and to present and interpret hydrogeochemical data.
- JNC/Golder' alternative modelling approach used all the chemical variability of the dataset, thus increasing confidence in the quality of the calculated groundwater mixing proportions.
- Posiva/VTT's mixing proportion calculations using different end members also provided a satisfactory, although time-consuming, alternative approach.

6.1.3 Hydrodynamic modelling

- Most groups were successful in calibrating and testing their respective models to simulate the Äspö groundwater flow conditions.

- Hydrogeochemistry, in the form of single chemical species or M3 mixing ratios, was used mainly to calibrate and modify properties of the HCDs.
- Flow paths to control points were to some extent shown and discussed. Only limited attempts were made to estimate the advective groundwater travel time distribution to the control points.

6.1.4 Hydrogeochemical modelling

- All groups treated the groundwater mixing ratios in the hydrodynamic simulations as conservative, i.e. assuming no water/rock reactions.
- Hydrgeoochemical modelling was attempted by six out of the nine groups.
- Hydrogeochemical reaction modelling, assuming thermodynamic equilibrium conditions, was carried out by four groups. Generally this showed that certain reactions had some effect on the groundwater chemistry during mixing. The reaction types tend to be site-specific, i.e. organic decomposition leading to an increase of HCO_3 is microbially mediated and takes place under the landmass; sulphate reduction, also microbially mediated, occurs under the sea floor. Cation exchange by clay minerals is significant suggesting an exchange of Ca/Na for Mg/K; such reactions are restricted to the presence of clays/gouge material in fracture zones and not considered widespread in the Äspö bedrock.
- However, hydrogeochemical reactions, whilst present, are largely overshadowed at Äspö when compared to mixing processes.

6.1.5 Integration of hydrogeological and hydrogeochemical modelling

- Simple simulation of mixing ratios (with or without chemical reactions) was used as a basis to calibrate (consistency check) the hydrogeological model
- Hydrogeochemical time-series data at the selected control points can reflect changes in the hydrodynamic flow conditions and were useful therefore for calibration purposes.
- Use of salinity (density) data to simulate large-scale hydrodynamic flow conditions was considered essential by some groups.
- Coupled flow and multicomponent reactive transport modelling were carried out by two groups; this is an important area to be developed.
- Modelling and integration strategies were to some extent discussed and described.

6.2 Understanding the Äspö Site

What additional insight has Task 5 provided in further understanding the dynamics and evolution of the groundwater flow system at Äspö?

The provided major hydraulic features (HCDs) appear to have been relevant and consistent concerning hydraulic responses. There was, however, one exception. Responses from the inflow to the shafts indicated the presence of a previously unknown fairly transmissive feature intersecting, or hydraulically well connected to, the shafts.

Was hydrogeochemistry successfully integrated in the hydrodynamic modelling exercises? What is the future of hydrgeoochemical and hydrogeological integration?

The modelling integration of hydrogeochemistry and hydrogeology has been largely successful given the time and resources made available; the following points can be emphasised:

- A common approach was to derive a calibrated hydrodynamic model based on hydrogeology. This model was then used to predict the chemical distributions and then recalibrated in some but not all cases to the measured chemical values by varying the fracture properties and boundary conditions.
- In some of the modelling carried out the travel velocity was poorly predicted. The hydrogeochemical data provided the opportunity to refine these velocities.
- The use of hydrogeochemical data was required to calibrate the model and also the aperture and storage parameters.
- Geochemical reaction modelling to quantify the influence of reactions on the groundwater chemistry during mixing can be used as a means to exclude locations were reactions are important, so that only locations characterised by mixing are compared.
- Confidence in a reliable hydrogeochemical conceptual model is another critical factor when initially deciding the boundary conditions to model the system.
- The future direction of hydrogeochemical integration should include further refinement of its use as demonstrated in the Task 5 modelling approach, for example:

    - helping to constrain initial and boundary conditions
    - providing reference water mixing proportions for time-series samples collected at hydraulically strategic localities

6.3 Site characterisation implications

What experience/knowledge gained from Task 5 can be successfully transferred to the site characterisation programme?

Several important implications of relevance to site characterisation were identified:

- Important to have a regional scale sampling strategy to collect data for the definition of initial and boundary conditions with reasonable resolution, i.e.:
    - Important to have good initial ideas of processes to guide the sampling strategy.
    - Important to obtain undisturbed and representative groundwater samples (i.e. not disturbed by drilling or other borehole activities prior to sampling)
    - Important to have a strategy for reasonable sampling time and space for ‘complete hydrochemical characterisation’ and a denser sampling programme in space for a limited number of chemical species.
    - Identify possible conservative tracers that should be sampled systematically in space and time.
    - Hydrogeochemical and hydrogeological data from deep boreholes at some distance from the repository site may be essential for setting up a reliable regional

descriptive geoscientific model that allows the interpolation and extrapolation of data to generate necessary boundary conditions in numerical groundwater/hydrogeochemical flow models.

- Important to judge what can be considered as a large scale model (regional model?) to test a geoscientific model description in a similar way as Task 5. This has implications for the above issue to define initial conditions at the site and regional scales. The first drilled boreholes are most likely to be distanced far enough apart to be unaffected by downhole investigations in the boreholes. However, when additional boreholes are drilled more closely together, as will be the case in the later stage of siting the repository, a more mixed groundwater situation might be encountered due to hydraulic tests and other activities in the boreholes. At least some data might then be considered less valuable than the early samples.

- Important to have a sampling strategy during repository construction to collect data for the definition of the transient conditions with a reasonable resolution, i.e.:
    - Try to take samples ahead of the tunnel excavation at a representative point near the tunnel; when the tunnel chainage has passed this point the sampling programme should be thorough and intensive during the first months followed by a less frequent sampling programme. Time-series sampling at key points should be identified before excavation by evaluation of hydraulic simulations and the hydrogeochemical description of the site
    - Have a reasonable sampling programme of 'complete hydrogeochemical characterisation' (or nearly the complete programme) at identified localities which are considered to be hydrodynamically connected to the key points along the tunnel
    - Have a reasonable sampling programme of 'complete hydrogeochemical characterisation' at identified points, which are at some distance from the excavated tunnel system.

6.4 Repository Performance Assessment (PA) implications

What experience/knowledge gained from Task 5 can be successfully transferred to repository performance assessment issues?

Although the modelling groups were not expected to discuss their results with reference to performance assessment (PA) implications, such a general discussion was implicit in the Task 5 rationale and this section attempts to address this issue.

A key requirement from a repository performance assessment is a description of radionuclide release and transport from a leaking defective canister in the near-field, into the geosphere and eventually to the biosphere. This description should be based on sound knowledge of the repository site geology, rock mechanics, rock thermal properties, hydrogeology, hydrogeochemistry and the transport properties (e.g. sorption, co-precipitation, immobilisation, diffusion etc.) of the geosphere and also the surface ecosystems. Therefore, the conceptual models and process descriptions for these individual disciplines which will eventually comprise the overall Geoscientific Site Descriptive Model (i.e. the complete description of conceptual models and geological evolution model as well as geometries of geological domains with their properties) will provide an important basis for determining the overall confidence in the system or site in question. However, maximum confidence, reliability and justification can only be obtained by integrating/coupling these disciplines and judging their consistency. To some extent geology and rock mechanics are intrinsically coupled, and to a certain extent also geology and hydrogeology. What Task 5 has attempted to address is to integrate hydrogeology with hydrogeochemistry.

The onset of Task 5 coincided with an OECD/NEA Workshop on the 'Use of hydrogeochemical information in testing groundwater flow models' (*OECD/NEA, 1997*), where the present status and future direction of integrating hydrogeochemistry and hydrodynamics was discussed, with particular reference to repository performance assessment. It was emphasised that to conduct a repository performance assessment required detailed near-field model(s), geosphere model(s) and biosphere model(s), and underlined the importance of constructing the geosphere and groundwater flow model(s) at various scales (i.e. regional, local and block scales). As summarised by *Gautschi et al. (1997):*

- Regional Scale: Determination of the general pattern of the flow system (e.g. identification of potential exfiltration zones), and definition of boundary conditions for the smaller scale models. Porous media groundwater flow models are commonly used, although some model variants incorporate major hydraulic features.
- Local Scale: Influence of the repository on the groundwater flow system (e.g. hydraulic gradients; water fluxes) by excavation of tunnels and shafts and the effects of tunnel and shaft seals. Porous media groundwater flow models are commonly used, although some model variants incorporate major hydraulic features.
- Block Scale: Entails a more detailed evaluation of groundwater flow heterogeneity in fractured rocks. Fracture network or channel network models are commonly used.

The degree to which hydrogeochemistry has been used in modelling at these scales also was summarised:

- Site Descriptive (Conceptual) Models: Hydrogeochemical and isotopic information; simple consistency check.
- Regional Scale Model: Regional distribution of hydrogeochemical parameters to demonstrate consistency of groundwater flow patterns; potential of groundwater residence times and past climatic conditions for independent model validation – however, only semi-quantitative because of too many uncertainties. More efforts will be necessary in the future to take into account solute transport processes and increase process understanding.
- Local Scale Model (repository scale): Pre-excavation phase with emphasis on borehole investigations leading to the identification and characterisation of major hydraulic fracture zones and rock mass areas of low permeability; post-excavation phase with emphasis on the characterisation of inflows/seepages (i.e. high/low hydraulic features) to the tunnel/shaft excavations (allows model testing and refinement); hydrochemical time-series monitoring of inflows to test groundwater mixing models.
- Block Scale Model (cavern/tunnel scale): Model testing and refinement basically similar to the local scale.

Also addressed was the issue of long-term evolution of groundwater systems as a basis of predicting future repository conditions. For example, modification of topography caused by erosion and the influence of glacial events (e.g. glacier movement and permafrost) will cause complex hydrodynamic changes. Integrated hydrogeochemical information, in terms of interpreting palaeo-events, plays a key role in predicting and modelling long-term hydrochemical and hydrodynamic stability of potential repository sites.

One final comment from the meeting: 'Logical reasoning, taking into consideration independent evidence from hydrochemistry, will enhance confidence in a safety case, but more effort is often needed to highlight this aspect in safety- and performance-assessment reports' (*Gautschi et al., 1997).*

Task 5, therefore, was initiated at a very opportune time and many of the PA-related issues considered above naturally formed an integral part of the Task 5 scope and objectives. The major question now to be addressed is whether Task 5 has made any significant progress to integrate hydrogeochemistry in PA-related hydrodynamic models? In terms of direct application of Task 5 models to a PA model chain of the type used in the SKB SR-97 safety case, it is not valid. However based on the accomplishments from the various modelling groups summarised in sub-section 6.1.5), there are some examples of modelling exercises that could be used in consistency checks and confidence building to show that the geosphere is reasonably well described, a necessary prerequisite for PA modelling. There are, of course, other PA modelling issues not considered in Task 5, for example possible flow paths and transport times from a repository to the biosphere based on alternative descriptive-model assumptions. Similar models, but more developed than those used in Task 5, could be used to calculate these flow paths and transport times as well as the long-term evolution of the groundwater system.

As a general conclusion from the Task 5 excercise, the use of hydrogeochemistry in safety and performance assessment would seem to be mainly relevant to: a) the development of site-descriptive (and conceptual) models at all scales, b) independent, consistency checks, and c) predict hydrogeochemical conditions at repository depths over repository timescales. Future progress should involve the continued development of coupled flow and reactive transport models which can improve the integration and testing of PA-related models, and also more use of hydrogeochemical transient scenarios.

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Appendix 1: Task 5. Data deliveries and summary of data usage

Judgement of data usage:

P = data of great importance for quantitative estimation of model parameters
p = data of less importance for quantitative estimation of model parameters
M = data of great importance used qualitatively for setting up model
m = data of less importance used qualitatively for setting up model
X = data useful as general background information
- = data not used

Summary of data usage (Importance of data; see notes first page)

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
1	Hydrochemical data 1	-	-			-	P			
1a	Surface bore holes-undisturbed conditions, Äspö-Laxemar	-	-		P		P	m	P	P
1b	Surface bore holes-disturbed conditions (by tunnel excavation), Äspö	-	-		P		P	m	P	P
1c	Surface bore holes-undisturbed conditions, Ävrö	-	-		-		P	m	X	P
1d	Surface bore holes-sampled during drilling, Äspö	-	-		P		P	m	X	M
1e	Data related to the Redox experiment	-	-		-		P	-	P	P
1f	Tunnel and tunnel bore holes- disturbed conditions	-	-		P			m	P	P
										P
2	Hydogeological data 1	M	P M							
2a1	Annual mean air temperature	-	-		X	-	-	-	-	-
2a2	Annual mean precipitation	X	p	M	p	X	-	p	-	M
2a3	Annual mean evapotranspiration	X	p	m	X	X	-	p	-	M
2b1	Tunnel front position by time	M	P M	P	P	M	P	P	P	P
2b2	Shaft position by time	M	P	P	p	M	P	P	P	P
2c1	Geometry of main tunnel	M	P	P	P	M	P	P	P	P
2c2	Geometry of shafts	M	P	P	p	M	P	P	P	P
2d	Hydrochemistry at weirs (Cloride, pH, Electrical conductivity, period: July 1993- Aug 1993)	-	-		p	-	p	-	-	-
2e	Geometry of the deterministic large hydraulic features (Most of them are fracture zones)	M	P	P	P	M	P	P	-	P

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
3	Hydrogeological data 2	P								
3a	Monthly mean flow rates measured at weirs. Tunnel section 0-2900m, period May 1991 – January 1994	P	P		P	M	P	P	-	P
3b	Piezometric levels for period June 1st 1991 – May 21st 1993. Values with 30 days interval (Task 3 data set)	-	P	P	P	X	P	P	P	P
3c	Salinity levels in bore hole sections for period -Sept 1993. (Task 3 data set)	-	M	M	-	-	-	-	P	M
3d	Undisturbed piezometric levels	-	p		p	-	P	p	P	P
3e	Co-ordinates for bore hole sections	m	p	P	P	P	P	P	P	P
3f	Piezometric levels for period July 1st 1990 – January 24st 1994. Daily values.	-	Pp	M	P	P	P	P	-	p
4	Hydochemical data 2	P	PM		-	-				
4a	Chemical components, mixing proportions and deviations for all bore hole sections used in the M3 calculations	-	P		-		P	X	P	P
4b	Bore holes with time series, > 3 samples (part of 4a)	-	P		-		P	p	-	P
4c	Bore holes sections interpreted to intersect deterministic large hydraulic features (Most of them are fracture zones) (part of 4a)	-			-		M	X	-	P
4d	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Undisturbed conditions	-	P		-		P	p	P	m P (in M3)

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
4e	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Disturbed conditions (by tunnel excavation)	-	P		-		P	X	-	m P(in M3)
4f	Boundary and initial conditions. Chemical components, mixing proportions and deviations (1989). Grid data for vertical boundaries based on interpolation. Undisturbed conditions	-	PM		-		P	p	P	m P(in M3)
4g	Boundary conditions after tunnel construction (1996) Chemical components, mixing proportions and deviations. Grid data for vertical boundaries based on interpolation. Disturbed conditions (by tunnel excavation)	-	P		-		P	X	P	m P(in M3)
5	Geographic data 1	m								
5a	Äspö coast line	m	-	M	M	M	M	P	P	P
5b	Topography of Äspö and the nearby surroundings	-	-	P	m	-	M	m	p	P
6	Hydro tests and tracer tests	-	-			-				
6a	Large scale interference tests (19 tests)	-	-		-		-	X	-	P
6b	Long time pump and tracer test, LPT2	-	-		-	p	-	-	-	-
7	Hydochemical data 3, update of data delivery 4 based on new endmembers. Recommended to be used instead of 4.	P	-		P	P				
7a	Chemical components, mixing proportions and	P	-		P	P	P	P	P	- p (in M3)

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
	deviations for all bore hole sections used in the M3 calculations									
7b	Bore holes with time series, > 3 samples (part of 7a)	-	-		P		P	P	-	P
7c	Bore holes sections interpreted to intersect deterministic large hydraulic features (Most of them are fracture zones) (part of 7a)	-	-		P		P	X	-	P
7d	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Undisturbed conditions	P	-	P	P		P	p	P	P
7e	Chemical components, mixing proportions and deviations. Grid data based on interpolation. Disturbed conditions (by tunnel excavation)	P	-		p		P	X	-	P
7f	Boundary and initial conditions. Chemical components, mixing proportions and deviations (1989). Grid data for vertical boundaries based on interpolation. Undisturbed conditions	-			P	P	P	p	-	m
7g	Boundary conditions after tunnel construction (1996) Chemical components, mixing proportions and deviations. Grid data for vertical boundaries based on interpolation. Disturbed conditions (by tunnel excavation)	-			p	p	P	X	-	m
										m
8	Performance measures and reporting 1					P				

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
8a	Performance measures				M	P		M	P	
8b	Suggested control points. 6 points in tunnel section 0-2900m and 3 point in tunnel section 2900-3600m.	-			M	P	M	M	P	P
8c	Suggested flowchart for illustration of modelling				M	-	X	m	P	m
9	Hydrogeological data 3	p				M				
9a	Monthly mean flow rates measured at weirs. Tunnel section 0-3600m, period: May 1991- Dec 1996.	p		P	P	M	P	P	P	P
10	Geographic data 2					-				
10a	Topography of Äspö and the nearby surroundings (larger area than 5b)	m			M		-	-	M	P
10b	Co-ordinates for wetlands	-	-		-		-	-	-	-
10c	Co-ordinates for lakes	-	-		-		-	-	-	-
10d	Co-ordinates for catchments	-	-		-		-	-	-	-
10e	Co-ordinates for streams	-	-		-		-	-	-	-
10f	Co-ordinate transformation Äspö system- RAK	m	-		X		-	-	-	-
11	Boundary and initial conditions	P				-				
11a	Pressure before tunnel construction, from the regional SKB model (TR 97-09)	P	M		m		M	M	-	P
11b	Salinity before tunnel construction, from the regional SKB model (TR 97-09)	-	M		m		m	P	-	P
11c	Pressure after tunnel construction, from the regional SKB model (TR 97-09)	P	M		m		M	X	-	P
11d	Salinity after tunnel construction, from the	-	M		m		m	m	-	P

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
	regional SKB model (TR 97-09)									
12	Performance measures and reporting 2					-				
12a	Suggested control points. 6 points in tunnel section 0-2900m and 3 point in tunnel section 2900-3600m (same as 8b) and 2 outside the tunnel.	-			M		M	P	P	P
13	Transport parameters compiled	-				X				
13a	LPT2 tracer tests	-	P		X	X	P	X	-	-
13b	Tracer test during passage of fracture zone NE-1	-	-		X	X	P	X	-	-
13c	Redox tracer tests	-	-		X		P	-	-	-
13d	TRUE-1 tracer tests	-	-		X		P	X	-	-
14	Hydrochemical data 4		-			X				
14a	Groundwater reactions to consider within TASK5 modelling (Description of how M3 calculates the contribution of reactions and identifying dominating reactions based on the M3 calculations.	x			X		X	X	M	P (in M3)
15	Co-ordinates for the test sections defining the control points	M		P	P	-	P	P	P	P
16	Co-ordinates for bore holes drilled from the tunnel	x			P	-	P	X	-	P
17	Hydrogeological data - prediction period	-								
17a	Hydrochemistry at weirs (chloride, pH, electrical conductivity, period: July	-			P		P	X	-	-

Data del. No	**Data**	**ANDRA/ANTEA**	**ANDRA/CEA**	**ANDRA/ITASCA**	**BGR/BMWi**	**CRIEPI**	**ENRESA/UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/Intera**
	1993 - Dec 1995)									
17b	Piezometric levels for period July 1st 1990 – Dec 1996. Daily values.	-			P		P	X	-	m
18	Hydrochemical data - prediction period.	-								
18a	Chemical components, mixing proportions and deviations for all borehole sections used in the M3 calculations. Data for tunnel section 2900-3600m.	-			P		P	P	P	P
18b	Boreholes with time series, > 3 samples (part of 18a)	-			P		P	P	-	P
18c	Borehole sections interpreted to intersect deterministic large hydraulic features (Most of them are fracture zones) (part of 18a)	-			P		P	X	-	P
19	Comments on tritium values									
20	Coastline, roads, grouting etc.									
	Other data (part of data in Task 1, 3 and 4)	-			X		X			
	Fracture orientation, fracture spacing and trace length – tunnel data		M		P		-	P	-	P
	Fracture orientation, fracture spacing– mapping of cores		M		-		-	P	-	P
	Fracture orientation, fracture spacing and trace length – mapping of outcrops		M		-		-	P	-	P
	Only POSIVA:Groundwater									

Data del. No	Data	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
	table over the Äspö island									
	Only ENRESA: The Redox Zone complete chemical database, including major, minor, trace and isotopes.									
	Only ENRESA: A surface recharge to the deeper aquifer of 5 mm/year. Inside the range proposed and published at several reports and scientific papers.									

Appendix 2: Task 5. Executive summaries of the individual modelling studies

(Abstracs, summaries or conclusions copied from each report)

Executive summary: ANTEA

In May 1999 ANDRA invited ANTEA to join the Task 5 of the ÄSPÖ HRL, more than a year after the beginning of this task.

The objective of this study is to simulate the hydrogeological and hydrochemical impact of the tunnel and shaft construction on the groundwater in the Äspö site and to compare the simulation results with measured data. The main results in this final report are dealing with sensitivity analysis and a general method to improve evaluation of the impact linked to the use of chemical data.

Earlier work in Task 1 of the Äspö HRL concerned model construction and first prediction of impact using only hydrological data to calibrate heads. The model developed for the purpose of Task 5 is a Mixte Hybrid Finite Element (MHFE) double porosity model taking into account the fracture network and the surrounding rock matrix. The fractures are explicitly modelled in 3D, each of them having their own parameter values. The rock matrix is considered as a porous media; a "high" permeability zone (SRD 4) is separated from the "mean rock matrix".

The extension of the model reproduces the volume on which all types of data are available (hydrogeological and hydrochemical); this is the volume used in the M3 (Multivariate, Mixing and Mass balance) calculations.

A quick sensitivity analysis was made to adjust the deep recharge and permeability of each fracture and rock matrix zone. For transient modelling we have chosen to commence calculations following the stop at tunnel front at 2600 m (December 1993) and to end the exercise at the beginning of May 1995.

After an encouraging first result, a complete sensitivity analysis was made over the main parameters defining as well the general hydraulic and transport conditions.

Analysis of the general conditions has given important information about mathematical conceptualisation and data treatment :

- The rock matrix can account for 5 to 10% of the calculated concentrations.
- Due to a fine geometric discretisation and a high dispersivity value, time step duration is not a real issue.
- The way initial data are interpolated can modify significantly the results.
- The uncertainty on M3 concentration is not implying significant bias in the concentration results.

Analysing the hydraulic and transport parameters has resulted in:

- Calculated concentrations are very sensitive to fracture permeability changes.
- Even though the model is quite large, the boundary conditions in heads have a very sensitive effect on the results.
- Kinematic porosity, specific storage and dispersivity have a sensitive effect on calculated concentrations, but in a less important manner.

To "calibrate" the model in terms of concentration, we have used the results of the sensitivity analysis and added all the changes leading to major improvements (i.e. use 0 MASL as a constant head boundary, multiply dispersivity by 2, multiply kinematic porosity and specific storage of NE-2, NE-4 and NNW-7 by 10). The optimised model based on the 4 end-member concentrations shows a 0.11 mean error, that compares very well with an uncertainty of ±0.1 in the M3 data.

Executive summary: ANDRA/CEA

This report is part of the work performed for ANDRA concerning flow and transport mechanisms in natural fractured media.

We present here the contribution of CEA/DMT to Task 5 of the TASK FORCE SKB. This task aimed at integrating groundwater flow models as well as hydrochemical mixing models for the situation at the Äspö site during the excavation of the tunnel and shafts.

The work performed includes modeling the hydraulic problem as well as the transport and mixing of different types of water within the conducting features at the site. The calibration approach followed corresponds to looking for a best solution to the problem and includes sensitivity analysis to appreciate the uncertainties in the calibration procedure.

However, since CEA/DMT only joined the Task 5 in April 1999, the work performed could only include partial calibration and sensitivity analysis for the different parameters of the system. Further work is required, mainly for the transport part of the model.

General conclusions

Results for the hydraulic problem show that hydraulic data provided (conductor domain geometry, transmissivities, boundary conditions) are fairly consistent. Density effects connected with salinity proved important for deeper parts of the model and should be modeled.

Incorporation of transport data allows for further refinements of the model although transport parameters as well as mixing proportions data involve large potential uncertainties. Preliminary results show that the system is sensitive to parameters like initial and boundary conditions as well as transport parameters (particularly dispersion coefficients). This should be taken into account in the calibration strategy as well as in the discussion about the global consistency evaluation of the modeling.

Comments to the modelling

For the hydraulic problem, good consistency level could be achieved for the model implemented. Nevertheless, the best solution provided is not unique as shown by sensitivity analysis conducted throughout the calibration.

Incorporation of mixing proportion data into the model allows for its refinement in the sense that hydraulic calibration of the system requires improvement. Nevertheless, preliminary results based on sensitivity analysis show that further level of uncertainty are introduced taking transport data into account. These involve uncertainties in transport parameters as well as calibration data like mixing proportions obtained from M3 based on scarce measurements.

Our present level of work on the system does not allow for conclusions on global consistency of the model including hydraulic as well as transport data. Nevertheless, uncertainty concerning transport parameters as well as data are important and should be taken into account in the analysis and the calibration strategy.

From a numerical point of view, this work will leads us in the future to develop and implement in CASTEM2000 the mixed hybrid finite element formulation for flow and transport in fractured network, fractures being 2D objects. Particle tracking procedure will be adapted as well.

Executive summary: ANDRA/ITASCA

Objective

The ANDRA/Itasca team participated in Task 5 for the purpose of gaining experience on modeling for a real site, and a first limited approach to coupling of transport and geochemistry. The issues of interest were:

- How can geochemistry help to improve the reliability of the hydrogeological modeling?
- What kind of complexities are added by looking at geochemistry and hydrogeology at the same time?

Approach - Modeling choices

After a model was constructed, it was first calibrated based upon water flow computations only. The model was then recalibrated using geochemical data. This is a discrete fracture model, with channelized flow in fractures. We consider Darcy's flow, with no density effect. The 21 fracture zones (Hydraulic Conductor Domains) as given in the data set are taken into account, whereas rock outside fracture zones is not modeled. The fracture zones are represented as planes, bounded either by the model boundaries or by planar boundaries as specified in the database. In each fracture plane, flow and transport occur along "channel pipes", i.e. a regular grid of one-dimensional elements. The grid has channels intersecting each other in four directions ("squares + diagonals" grid), at 45° angles.

Transmissivity, width, and storage coefficient are constant for each feature, except at the top boundary under the Baltic, where a "skin factor" is used. The transmissivity values are initialized from the data set, then changed during calibration phase. The specific storage is used as given when data are available (NE-1, NNW-1, NNW-2), and computed from the correlation in TR 97-06 for all other fracture zones. The boundary conditions are:

- Constant flux under land, and constant head (with skin factor) under sea at the top surface;
- Constant head on vertical faces;
- No flux on the bottom face.

The hydraulic calibration is performed by imposing the flow rates in the tunnel and trying to reproduce the available drawdown histories in boreholes. The calibration parameters are the transmissivities in fracture zones.

Conservative transport is modeled by advective / dispersive particle transport, with spreading due to both longitudinal dispersion in channels and to complete mixing at channel intersections. For end-member simulation, the initial mixing ratios in each channel are interpolated from the cubic-grid interpolation at the start of the period, as provided in the database. These mixing ratios are maintained constant on vertical boundaries throughout the simulation. For the top boundary, we use pure meteoric water under land and pure Baltic water under sea.

Mixing ratios at the control points are then used to calibrate the skin factor at the bottom of the Baltic Sea. The final skin factor we use is 100, i.e. we add at the bottom of the sea, above each fracture zone, a 10m-thick layer with a transmissivity equal to 1/100 of the mean fracture zone transmissivity.

Overall, the final model after calibration is relatively close to the initial one. Fracture zone NE2's transmissivity needed a 100-fold increase. This may mean there is another unknown conductor in its vicinity. Otherwise, only NNW1 (divided by 10) and NNW3 (multiplied by 10) had to be modified significantly.

Modeling results

Sensitivity studies were performed by doing simulations with modified parameters, testing:

- The effect of the chosen discretization (grid size from 40m to 80m, with either square grids or "four directions" grids.
- Fracture zone hydraulic conductivities (calibration procedure - both "bulk conductivities and skin factor under Baltic sea).
- Fracture zone specific storage (from no storage to ten time the chosen one).
- Longitudinal dispersivity (tenfold increase).

The simulation results had a very small sensitivity to discretization. The hydraulic conductivities used had a high influence on flow patterns, whereas specific storage was not very influential, with relatively fast piezometric response to the tunnel advance. Similarly, dispersion in the model was dominated by the mixing at intersections, so that the longitudinal dispersivity had little effect.

The simulations tend to overestimate the amount of Baltic water arriving at the Control Points, despite the skin factor we use at the bottom of the Baltic Sea. Note that for simulations performed after hydraulic calibration only, the overestimation is much larger.

Coupling with geochemistry

Fully coupled reactive transport was simulated on a part of the model domain only. We did not use the endmembers provided by the Task Force, but directly dealt with chemical species. For some species, concentrations had to be derived from endmember mixing ratios and endmember compositions.

The simulated geochemical processes included solution complexation, precipitation / dissolution of minerals and gas dissolution (CO_2) for those of the nodes opened to the atmosphere.

The simulations performed show some interesting potential features about coupling transport with geochemistry. For example, in the context of the Äspö island, it appears that variable water salinity influences the aqueous solution ionic strength and consequently the "apparent" chemical reaction constants.

Conclusions

Using flow results only to calibrate the transmissivities of the Hydraulic Conductor Domains proved to yield non-unique results. However, by looking at chemical transport, we were able to calibrate the flow parameters in a better way, by adding more constraints to the calibration process. Overall uncertainties remain quite large. Specifically, the interpolation of the initial chemical compositions we used is not satisfactory, and the influence of the not-well-known fixed-concentration lateral boundary conditions has a large impact on the final results. Reactive transport results show that, even in zones where geochemistry is considered as simple and of little importance (e.g. in the absence of significant redox or surface reactions), transport of chemical species might in fact be affected by mineral precipitation / dissolution, therefore constraining the hydrogeological modeling.

Executive summary: BMWi/BGR

This study deals with the influence of the tunnel construction on the groundwater system at the Äspö site and looks at changes in the flow pattern as well as the disturbance of the chemical balance. Hydraulic and transport models were constructed to simulate the dominant hydraulic and chemical processes in the investigated area with and without the spiral tunnel.

Flow and transport calculations were carried out with a multi-fracture model including fracture zones NE-1, NE-2, NE-3, NE-4, EW-1 78°, EW-1 88°, EW-3, NNW-2, NNW-4, and NNW-7 belonging to the regional fracture system. The conditions before, during and after tunnel construction were simulated. Measured piezometric heads and the distribution of the four water types: meteoric, Baltic Sea, glacial, and brine at different control points were compared to simulated values. Model parameters were varied corresponding to the deviations to achieve a better match between the measured and simulated values.

The flow modelling confirmed the observed drawdown beneath the island of Äspö and the resulting change in the flow pattern and flow velocities. In contrast to initial conditions, the model indicates downward groundwater flow above the tunnel and upward flow in the fractures beneath the tunnel. Conservative transport calculations demonstrate the changing mixing ratio of groundwaters of different origin at the site (meteoric, Baltic sea, glacial, brine water). This effect can be compared to observed chemical compositions at specific control points. The change of the flow directions owing to the drawdown results in dilution of dissolved substances by meteoric water flowing into the aquifer. The upward groundwater flow of brine increases the salinity in the deeper part of the investigated area.

Chemical analyses of non-conservative elements in the water samples show a clear deviation compared to simulated concentrations from the mixing model. For this reason, different approaches were pursued to identify chemical processes and to increase the understanding of the groundwater changes associated with tunnel excavation. A general conceptual model of the essential hydrochemical conditions at the site during the tunnel excavation was composed. Chlorine, Bromine and also Sodium behave conservatively and can largely be reproduced by a pure mixing approach. In general, the groundwater components SO_4^{2-}, HCO_3^-, K^+, Ca^{2+}, and Mg^{2+} are affected by chemical processes. Cations are for the most part controlled by exchange processes. Sulphate, hydrogen carbonate, and calcium are influenced by dissolution and precipitation of calcite and gypsum. Additionally, organic redox reactions and organic decomposition may account for the observed carbonate and sulphate chemistry. Nevertheless, it can be assumed that a few chemical reactions, that influence the groundwater composition, cannot be identified because of different processes that lead to opposite effects concerning loss or gain of elements.

Executive summary: CRIEPI

The groundwater flow and geochemical distribution were simulated during tunnel construction around Äspö. The stabilities of selected geochemical components were investigated by using PHREEQE.

A unsteady state of groundwater flow was simulated by considering the progress of tunnel and the change of inflow to the tunnel section. Excluding modeling the grouting and skin effect around tunnel, the inflow to the tunnel was expelled the inflow measured at tunnel section as flux boundary. Calibrations of transmissivity of the Hydraulic Conductor Domains (HCD) were also performed.

The progress of tunnel construction and the time series of drawdowns are quit useful to understand the hydrogeological model because these relationships clarify the impact and response. Drawdowns were roughly represented by properly modeling the geometric relationship between tunnel, shaft, HCD and monitoring borehole section.

The geochemical distribution of selected chemical components was simulated using the results of Multivariate Mixing Mass balance calculations (M3). The simulated mixing portions of old waters, i.e. Glacial water and Brine water, and sum total of fresh waters mixing portions, i.e. sum total of Baltic Sea water and Meteoric water agreed with the results of M3, but the ratio of fresh water, i.e. Baltic Sea water and Meteoric, water disagreed. Based on the simulated mixing portion, the deeper part of groundwater was replaced by Baltic Sea water rather than Meteoric water. According to the investigation by using PHREEQE, some geochemical components are sensitive to geochemical reaction. The further studies are needed to explain this inconsistency, for example, geochemical reactions, boundary conditions, local effect of sampling. However, the investigation focusing on the end-members is useful to understand the path of groundwater flow and the property of HCDs.

Concerning measured helium concentrations, the simulated helium concentrations are in good agreement with the measured concentration with few assumptions. Since measured and simulated results reflect the hydraulic properties of HCDs, it is a potentially useful method to verify the hydrogeological model.

Executive summary: ENRESA/UDC

The numerical modelling of the groundwater flow and solute transport of the Äspö site has been successfully performed.

The tunnel construction process has been simulated by means of 29 stages for the transient groundwater flow model. Flow rates into the tunnel are computed by the model and not prescribed as a boundary condition.

Computed flow rates show an excellent agreement with measured data in most of the tunnel sections. The comparison of the computed pressure heads and the measured values indicates that in general the numerical model is able to reproduce the measured drawdowns. Calibrated transmissivities are within the range of field measured values except for two of the 19 considered hydraulic domains, were a little lower transmmissivity value was calibrated. Finally, the groundwater flow numerical model has been succesfully validated against field data not used in the calibration stage.

Numerical results in terms of concentrations show an excellent agreement with measured data of chlorides and 18-oxygen. It is important to remark that solute transport results were achieved without calibration. With a strongly consistent (and calibrated) flow model, the numerical model reproduces conservative chemical concentrations using available transport parameters.

In order to assess uncertainty in initial and boundary conditions and parameters, a sensitivity analyses of the numerical model was done for groundwater flow and solute transport. Groundwater flow model is strongly sensitive to the initial conditions and transsmissivities of the Hydraulic Domains. On the contrary, the model is not sensitive to the parameters of the intersections among domains and with respect to the boundary conditions. Solute transport model is strongly dependent on initial conditions of concentrations. Initial concentration field was found as the most important source of uncertainty.

A good agreement was found between M3 model results and hydrodynamic numerical model of groundwater flow and solute transport. In general, it can be stated that a there is a consistency between both types of models. This consistency supports the hypothesis of the mixing of 4 extreme reference waters at the Äspö groundwater system, as proposed by M3 model. M3 results has been useful to shape some aspects of the Äspö site hydrogeology. However, the comparison of hydrodynamic and mixing models results must be taken carefuly, due to the combination of uncertainties on the mixing model (+/- 10%) together with the detected uncertainties in the interpolation of the mixing fractions further on the sampling points (+/- 10%).

Predictions at 3 of the 4 proposed prediction points have been made. They include a base run (best prediction) and a second run using an alternative initial concentrations field. The results of both runs provided a reliable prediction range which was in agreement with field measurements.

The role of the chemical reaction have been evaluated by means of comparison of computed results and measured concentrations of the typically non-conservative species. Sources of bicarbonate, calcium and sulphate have been clearly detected, which are assumed to be caused by chemical processes. A different behaviour of calcium and bicarbonates have been found depending on the location of the fracture zones. As a cualitative hypothesis, the carbonate system could be affected by the higher availability of Fe(III) expected under the islands. As proposed by Banwart (1999) for the Redox Zone, carbon oxidation through Fe(III) reduction could constitute a source of bicarbonates. This hypothesis (and other chemical behaviours which remains still unclear) can be quantitatively validated or rejected by means of coupled groundwater flow and reactive transport modelling.

Executive summary: JNC/GOLDER

Report 1998:

This report describes preliminary modeling to demonstrate the application of FracMan Discrete Feature Network and PAWorks Pathways Analysis software to support Task 5, site scale hydro-geochemical modeling of the Äspö HRL site.

The modeling was carried out based on preliminary project data, and will be updated during 1999. The analysis defined the sources of water breaking through to the Äspö tunnel through pathways defined from a 2 km scale discrete fracture network model. Water sources are based on an initial spatial distribution of geochemical end-members, which makes it possible to calculate the geochemical end-member breakthrough to each point within the Äspö tunnel. The modeled period was from 1990 through 1996.

The analysis included development of a novel approach to incorporate the effect of varying density on flow velocity, based on a synthesis of the concepts of environmental and freshwater heads.

Report 2000:

This report describes the participation of the JNC/Golder team in the coupled hydrogeological/geochemical pathway modeling of the construction of the Äspö Hard Rock Laboratory during the period 1990 through 1996. Modeling was carried out to the specifications of the Äspö Task Force on Modeling of Groundwater Flow and Transport of Solutes, Task 5. In order to demonstrate the value of geochemical data in hydrogeological modeling, models were calibrated separately to hydrogeological data and geochemical data. Both of these calibrated models were then used in predictive simulations.

Following these simulations an additional set of complimentary analyses were undertaken to address issues of uncertainty related to the geochemical methodology. Concurrently, the algorithm used to compute the source locations of the waters infiltrating into the tunnels was improved.

The modeling was carried out using the discrete feature network/channel network approach (DFN/CN). In this approach, both major deterministic fracture zones and background fracturing was modeled explicitly as two-dimensional discrete features using FracMan/FracWorks. Deterministic fracture zones were based on the zone specifications of Rhén (1999), with the addition of a northwest trending feature to explain the step drawdown responses observed during shaft construction.

Flow and transport were modeled by transforming the fracture network to a topologically equivalent pipe network using FracMan/PAWorks.

For the main simulations hydrological and geochemical initial conditions for the model were provided by SKB. All transport calculations were made using transport pathways defined by graph theory searches through the channel network model. The flow velocities were adjusted to account for the effect of salinity on density and flow (Bear, 1972). This density-corrected transport was expressed in terms of travel times and proportions of four geochemical end member water geochemistries: meteoric, glacial, marine, and brine. Oxygen-18 and chloride were back calculated from the geochemical end members. The modeled period was from 1990 through 1996.

For the additional complimentary Task 5 analyses, two major changes were adopted. Firstly, the geochemical initial conditions for the model were adapted to enable consideration of all the chemical variability in the measured data. Several possible alternative combinations of input data were considered. The second change was that the methodology for finding the source locations of the water types was changed from a graph theory search to a particle tracking approach. The latter provides a more accurate measure of the proportion of mass originating in a given location.

The three stages of the modeling process achieved differing levels of success. The purely hydrogeological model constructed in Stage 1 was very successful in matching the head distribution, but did not provide optimum geochemical predictions.

The Stage 2 geochemical calibration, using the M3 chemistry and the original pathway algorithm, involved additional changes to the boundary conditions and connectivity. In particular the geochemical data provided information on model where the model required additional/lower connectivity. The addition of geochemical information resulted in both lower head and geochemical error measures.

However, the most interesting results from the modeling occurred during the Stage 3 analysis. This model used an improved chemistry model and pathways algorithm, but was only run using the hydrogeologically calibrated fracture model and boundary conditions. Fits between the measured and modeled chemistry were very good: the deficiencies primarily being related to travel velocities, not spatial location. The results from this set of simulations indicate that for a large modeled region the initial geochemical spatial variation used in the model is very important.

In conclusion, the authors believe that the specific objectives of Task 5 were met. The first objective, “to assess the consistency of groundwater flow models and hydrochemical mixing-reaction models through the integration and comparison of hydraulic and hydrochemical data obtained before, during and after tunnel construction” was addressed. The model derived from purely hydrogeological considerations was adequate for determining the major connectivity of the system. However, the geochemical response was strongly influenced by the geochemical interpretation and optimization required additional calibration. The use of a geochemical conceptual model improved the geochemical interpretation. The use of geochemical data was also required to calibrate the model aperture and storage parameters.

The second Task 5 objective, “to develop a procedure for integration of hydrological and hydrochemical information which could be used for assessment of potential repository sites” is discussed in detail in Section 5-5 and 6. The approach is based on sequential use of the hydrogeological and geochemical data. The phases could be summarized as:

- Develop a regional model of the site including only the large scale features
- Develop a conceptual model for the background fractures. For a DFN idealization this included the orientation, size, intensity, and transmissivity of the non-regional features.
- Develop boundary conditions for the modeled region.
- Create a finite element model including the major features, background features, and boundary conditions. Calibrate this model to the measured head distribution by varying the fracture properties and boundary conditions.
- Use this calibrated model to predict chemistry distributions. Calibrate this model to the measured chemistry and head distribution by varying the fracture properties and boundary conditions.

Based on the Task 5 modeling of the Äspö site this approach worked well. It was found that the calibration to measured heads provided a reasonable calibration to the general water sources, but that the travel velocity was poorly predicted. The chemistry data provided a data set from which to refine these velocities. Chemistry data also reduced the non-uniqueness of the system.

It should be noted, however, that the goodness-of-fits achieved were also sensitive to the methodology used to compute the geochemical distribution across the site. The hydrogeology and the geology at the Äspö site are consistent with the major features dominating mixing and flows. Therefore it was necessary to distribute chemistry based on the major features, rather than assuming a continuum. The strong influence of the Baltic/Äspö Island boundary on the chemistry also markedly affected the interpretation. For a different site, this means that the modelers would need to ascertain the structures, geology and/or major processes affecting the chemistry prior to setting up the geochemical spatial distribution. Similarly, the interpretation scheme should also account for the hydrogeological conditions.

Executive summary: POSIVA/VTT

The Task #5 project was a part of the Äspö task force on modelling of groundwater flow and transport of solutes. The aim of the Task #5 was to compare and eventually integrate hydrochemistry and hydrogeology. At the launch of the project, it was stated that the results and methods developed in the project would be useful for an assessment of the stability of the hydrodynamic and hydrochemical conditions for any future repository site located in a crystalline bedrock environment. The first objective of the task was to assess the consistency of groundwater flow models and hydrochemical mixing-reaction models through comparison of hydraulic and chemical data as a function of Äspö tunnel construction. The ultimate objective was to develop a procedure for integration of hydrological and hydrochemical information.

The starting point for consistency comparisons, and integration of hydrological and hydrochemical information is how the mixing fractions and initial boundary conditions of the reference water types are extracted from the geochemical data. Two optional methods for this extraction were available. The results of the first method were delivered for all Task #5 modelling groups, and it classifies the geochemical data with reference of four different water types: brine (highly saline water), glacial melt (water from the Pleistocene glacier), meteoric (1960's precipitation estimate) and the present Baltic Sea water. Posiva Oy's modelling group developed the second method for geochemical data interpretations. The second method classifies the geochemical data with reference of seven different water types: saline, preglacial altered (shallow altered mixed water), glacial melt, Litorina Sea (relic fresh seawater), postglacial altered (shallow altered seawater), meteoric (shallow altered fresh water) and the Baltic Sea water (present fresh seawater).

The hydrodynamical modelling code, used in the flow-transport simulations, couples the residual pressure and salinity fields to solve the groundwater flow and solute transport equations defined for the study volume. Mixing fractions are transported in the simulations like any solute. No geochemical reactions are taken into account during transport. Initial conditions (hydrological and geochemical) on the boundaries and within the study volume give the starting values for the calculations. The consistencies between the simulated mixing fractions (groundwater flow model) and the observed mixing fractions (hydrochemical mixing-reaction model) at specific control points are attempted to reach by modifying hydrological parameters within the study model suitably. The second geochemical modelling method used in the studies allows assessment of net-geochemical reactions along a flow path after a simulation; fulfilling the hydrological-geochemical integration demand with a loose one-step process.

The two optional geochemical data extraction methods and the simulation results with the two alternative geochemical boundary conditions show significant discrepancies. Differences in results can be pointed to geochemical extraction methods and inadequate hydrological definition of the model volume. These discrepancies as such strongly point out the need of integrated view in repository site investigations.

Executive summary: SKB/CFE/Intera

Characterisation of a site for nuclear waste disposal normally involves development of hydrodynamical and hydrochemical numerical models. These models, and the basic data sets, are however in most cases developed independently, and may even be inconsistent. This report describes an attempt to integrate hydrological and hydrochemical information and modelling concepts.

The key element in this integration is the obtained chemistry calculated as mixing portions of water types by using a new modelling technique. This concept can be used in both hydrochemical and hydrogeological modelling of a site. The groundwater at Äspö is modelled to consist of a complex mixture of the water types: Meteoric (precipitation water), Baltic (seawater), Glacial (meltwater from the last glaciation) and Äspö Brine (old highly saline groundwater). The hydrochemical analysis, and model, gives the spatial and temporal distributions of these four water types. In the hydrodynamical model it is also possible to calculate the distribution of water types, for example by solving a number of advection/diffusion equations, provided that initial and boundary conditions are available (these are derived from field data by the hydrochemical analysis). The results from the hydrodynamical model, in particular path lines and flow velocities, can in turn be used in the hydrochemical analysis, as the transport aspect is normally missing in these models. From this brief description it is clear that an integrated view, based on both hydrogeological and hydrochemical information from a specific site, can and ought to be established.

The project was carried out along the lines indicated above and a number of comparisons and integrated evaluations were carried out. In this process both the hydrochemical and hydrodynamical models were “exposed in a new light”, stimulating new developments and improvements. An improved understanding of the studied site was also obtained in this process.

The general conclusion of the study is that the integrated view and evaluation, based on both hydrochemical and hydrogeological information, is of great value in a site investigation. The hydrodynamical models are constrained by new data sets and information and the hydrochemical models can benefit from the information concerning path lines and transport velocity.

Appendix 3: Task5. Summaries of the individual modelling concepts

Summary of the models for water flow calculations

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BMWi/BGR	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera (1)	SKB/CFE/Intera (2)
Type of model	Double porosity model : explicit 3D representation of matrix and fractures	Deterministic	Discrete fracture model, with channelized flow in fractures	Discrete fracture network	Determistic continuum model	Deterministic discrete fracture network model.	Stochastic Discrete Fracture Network (DFN) Model	Porous medium, dual porosity	Stochastic continuum model	Continuum model based on a fracture network
Process description	Darcy's equation	Darcy´s flow including density driven flow. (The coupling with salinity transport was made optional, calibration was done without coupling to save time). Transport of salinity fields.	Darcy's flow, no density effect	Transient saturated Darcy's flow disregarding density effects	Darcy's flow	Transient groundwater flow assuming Darcy's Law and neglecting density effects.	Transient flow solution using Darcy's flow equations.	Advection, dispersion, molecular and matrix diffusion Coupled flow and transport by density and Darcy velocity	Darcy´s flow including density driven flow. Adv/Diff equation for salinity Mass conservation Density function of salinity	Darcian flow including density effects Adv/Diff equation for salinity Mass conservation Density function of salinity
Geometric framework and parameters	Model size : size of the M3 model : 3.750x 2.520x1.500 km^3 Local fractures : Most of the deterministic local features, only EW-7 and NNW-3 are not represented. Regional fractures : SFZ-03, SFZ-04, SFZ-05, SFZ-07 (continuation of EW-1), SFZ-11, SFZ-12 (continuation of NE-1), SFZ-14 Rock Mass Domain : deterministic. Two	Model size 2x2x1km^3 Deterministic features: kept 16 : EW1S, EW3, EW7, NE1, NE2, NE3, NE4N, NE4S, NNW1, NNW2, NNW3, NNW4, NNW5, NNW6, NNW7, SFZ11. The other ones are not intersected neither by the above ones nor the tunnel and shaft. Rock outside the deterministic features is not modelled	Model boundaries, in Aspo coordinates: X = 1000 to 3000 Y = 6000 to 8000 Z = -1000 to 0 Deterministic features: the 21 fracture zones as given in the data set Rock outside fracture zones not modelled	2 x 1.8 x 1 km^3 A selection of 10 deterministic features provided in the data set (NE-1, NE-2, NE-3, NE-4, NNW-2, NNW-4, NNW-7, EW-1 78°, EW-1 88°, EW-3) Rock domain ignored between deterministic fractures	Model size: 2.0x2.5x1 km^3 . Easting 1000-3000m, Northing 5500-8000m, 0 - -1000m in depth at Aspo coodinate Determistic features: All except for regional structure, ex. SFZ03, SFZ12. Rock outside the deterministic features modelled as determistic continuum.	2 x 2 x 1 km^3 Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features neglected.	Model Size: N-S 2.0 km; E-W 2km; depth 1 km Deterministic features: All SKB deterministic features provided in the data set. In addition an additional "mystery feature" was added to match the drawdown responses. Deterministic BH features: features added through BH sections to improve connectivity BH to	Model size: cross-section hexahedron with diameter about 3.3 km, depth 1.5 km Fracture zones provided in SKB TR 97-06 Rock between the fracture zones Both the fracture zones and the rock between them modelled as dual porosity medium	Model size: 1.8x1.8x1 km^3 . Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features modelled as stochastic continuum with no correlation between the cells in the model.	Model size: 1.8 x 1.8 x i km^3 Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features modelled as continuum, based on a fracture network.

TOPIC	**ANDRA/ANTEA**	**ANDRA/CEA**	**ANDRA/ITASCA**	**BMWi/BGR**	**CRIEPI**	**ENRESA/UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/Intera (1)**	**SKB/CFE/Intera (2)**
	domains : SRD-4 is modelled independently						DFN model. Stochastic features: Background features modelled using stochastic discrete features.			
Material properties and hydrological properties	Fractures : Conductivity (K), specific storage (Ss) Rock mass domain : Conductivity (K), specific storage (Ss)	Deterministic features: Transmissivity (T), Storativity(S)	Transmissivity (T), width (W), storage coefficient (S)	Deterministic features: Permeability (K), Storativity (S), Fracture aperture (b) Rock domain ignored between deterministic fractures	Deterministic features: Transmissivity (T) Rock outside deterministic features: Hydraulic conductivity(K), Specific storage (Ss) is same in the modelling area	Deterministic features: Transmissivity (T), Storativity(S) Rock outside deterministic features: neglected	All features: Storativity (S) Aperture (A)	Fracture zones: Transmissivity (*T*), widths (*w*), storage coefficients (*S*), total porosity (□) as sum of kinematic porosity (ϕ_f) and diffusion porosity (ϕ_d) Rock between the fracture zones: Hydraulic conductivity (*K*), specific storage (S_S), total porosity (□) as sum of kinematic porosity (ϕ_f) and diffusion porosity (ϕ_d) Diffusion porosity (ϕ_d), fracture spacing (*2a*), matrix porosity (ϕ’), longitudinal ($\square_L$) and transversal ($\square_T$) dispersion lengths for the fracture zones and the rock between them	Deterministic features: Transmissivity (T), Kinematic porosity, Thickness Rock outside deterministic features: Hydraulic conductivity(K), Kinematic porosity	Deterministic features: Transmissivity (T), Kinematic porosity, Thickness Rock outside deterministic features: Hydraulic conductivity(K) Kinematic porosity

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BMWi/BGR	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera (1)	SKB/CFE/Intera (2)
Spatial assignment method	Fractures : constant properties within each features (T, Ss, Ne). Change of K for some features (SFZ-05, NE-2, NNW-7, NE-3, NNW-4, NE-4) du to calibration procedure. Rock Mass domain : constant properties within each zone (SRD-4, rest). No change	Deterministic features: Constant within each feature (T,S). T values were changed during the calibration. Grouting is taken into account.	Constant for each feature, except at the top boundary under the Baltic, where a “skin factor” of 0.01 is used. Transmissivity started from data set (*Source: HCD-SR97.XLS in Data Delivery 2*), then moved during calibration phase. Specific storage used as given when data available (NE-1, NNW-1, NNW-2, computed from correlation in TR 97-06 for all others	Deterministic features: Constant within each feature (K, S) Fracture aperture different within each fracture, e.g. at tunnel locations Rock domain ignored between deterministic fractures	Deterministic features: Constant within each feature (T). Transmissivity of NNW-7 changes twice value due to calibration, Transmissivity based on Table A2-7 and A2-8, TR97-06 Rock outside deterministic features: Unity value Before calibration, 1.5e-9m/s (3m-scale hydraulic permeability test) After calibration, 6.0e-9 m/s (3m-scale hydraulic permeability test)	Deterministic features: Transmissivity (T), Storativity(S) : Constant within each feature	Deterministic features: Constant within each feature (T,S,A). No changes in T due to calibration. Transport Aperture set at 2 $T^{0.5}$. Storativity baseline 0.001 $T^{1/2}$. S increased by: EW-1S – factor of 3 EW-3 (z<200) – factor of 3.2 NE-2 - factor of 3.3 NE-4N - factor of 3.5 NNW2 - factor of 1.5 NNW-8 - factor of 1.7 Mystery feature: T = 1.e-5 m^2/s. A = $2T^{0.5}$. S= 0.001 $T^{1/2}$. Background features: Orientation bootstrapped. T – LogNormal ($\mu = 9 \times 10^{-7}$ m^2/s, $\sigma = 5 \times 10^{-6}$ m^2/s). A = $2T^{0.5}$. S= 0.001 $T^{1/2}$.	Properties given for each element in the model Depth dependence for the transmissivity of the fracture zone EW-3 (both M3-based and inverse modelling-based simulations) and NNW-8, SFZ05 and SFZ12 (including NE-1) (the inverse modelling-based simulations only) Depth dependent fracture spacing Kinematic porosity calculated from the hydraulic conductivity/transmissivity and the fracture spacing	Deterministic features: Constant within each feature (T). Minor modifications due to calibration. Rock outside deterministic features: (K) lognormal distribution without correlation between the cells.	Deterministic features: Constant within each feature. Minor modifications due to calibration. Rock outside deterministic features. Transmissivities of background fracture network related to size of fracture. Hydraulic conductivity(K) for cells based on transformation from the transmissivities on the applied fracture network,

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BMWi/BGR	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera (1)	SKB/CFE/Intera (2)
Boundary conditions	Earth (island + continent) : constant flux. Change du to calibration. Sea + lake : constant head. Other external boundaries : Based on Swenson regional model. Tunnel and shaft : time varying fluxes.	Surface: Constant recharge on Aspo. Sea: Constant head Vertical : Head picked up from regional model by Svensson as well as salinity distributions Bottom: No flux.	Top surface: constant flux under land, and constant head (with skin factor) under sea. Vertical faces: constant head Bottom face: no flux	Surface: Constant flux Sea: Constant head Vertical-North: Fixed pressure Vertical-East: Fixed pressure Vertical-South: Fixed pressure Vertical-West: Fixed pressure Bottom: No flux Inner: Flow rates or constant heads respectively The water flux in the model is a function of the size of the cone of depression, which depends on the location of the tunnel	Surface: Constant flux in Aspo, Constant head in others that mean sea and island, ex. Laxmar, Halo and Mjalen. Side: Fixed pressure based on hydrostatic pressure. Bottom: No flux. Tunnel: time variable flux boundary, tunnel gain is expressed by hydraulic permeability chenge at line element.	Surface: Constant flux. Sea: Constant head Vertical-North: Fixed pressure equals to the initial one Vertical-East: Fixed pressure equals to the initial one Vertical-South: Fixed pressure equals to the initial one Vertical-West: Fixed pressure equals to the initial one Bottom: No flux.	Base: “no flow” boundary (= constant flux of 0.0 at each node) Sides: The sides of the model were specified as constant head values interpolated from the density corrected values of Svensson (1999). Surface of Äspö Island: was specified to have a constant infiltration rate of either 0.0 mm/year or 30.0 mm/year. Infiltration of 0 mm/year was used for final simulations. Baltic seabed: A constant head boundary condition of 0.0 m. Äspö tunnel: Tunnel prior to construction: group flow rate of 0.0 m3/s. Tunnel following section construction: flow rate equal to the measured inflow rate.	Land: zero salinity (M3-based simulations), chloride 0.1 g/l (inverse modelling-based simulations), initially and time step #1: groundwater table, time steps #2–#17: constant flow rate Sea: zero residual pressure, constant salinity (M3-based simulations) or constant chloride concentration (inverse modelling-based simulations) Vertical edges: residual pressure on the basis of a salinity (M3-based simulations) or chloride distribution (inverse modelling-based simulations), constant in time Bottom: salinity (M3-based simulations) or chloride concentration (inverse modelling-based simulations),	Top: Specified flux on land specified pressure and salinity below Baltic Sea. Vertical and bottom: From a regional model. Linear change by time based on regional simulations for undisturbed conditions and with Äspö tunnel present.	Top: Specified flux on land specified pressure and salinity below Baltic Sea. Vertical and bottom: From a regional model. Linear change by time based on regional simulations for undisturbed conditions and with Äspö tunnel present.

TOPIC	**ANDRA/ANTEA**	**ANDRA/CEA**	**ANDRA/ITASCA**	**BMWi/BGR**	**CRIEPI**	**ENRESA/UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/Intera (1)**	**SKB/CFE/Intera (2)**
								constant in time Tunnel and shaft: residual pressure and flow rate in each time step Residual pressure initially also in the interior and bottom nodes and concentration in the interior nodes, released in the first time step		
Numerical tool	TAFFETAS	CASTEM2000	3FLO	DURST / Rockflow	**FEGM**/FERM	TRANMEF-3	FracMan / PAWorks	FEFTRA	PHOENICS	PHOENICS
Numerical method	Mixte Hybrid Finite Element	Mixed and Hybrid Finite Elements Method	Finite Elements method	Finite element method	Finite element method	Finite Element Method	Finite Element Method	Finite element method	Finite volume method	Finite volume method
Output parameters	Head, Flow	Head, flow, concentration fields	Head, flow	Heads Flow field Flow velocity and corresponding amount of water	Head, Darcy's velocity	Head and Flow	Head, net flow at nodes, particle location with time.	Residual pressure and concentration fields	Head, flow and salinity field.	Head, flow and salinity field.

Summary of the models for tracer transport calculations

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera (1)	SKB/CFE/Intera (2)
Type of model	Double porosity model : explicit 3D representation of matrix and fractures	Deterministic	Discrete fracture model, with channelized flow in fractures	Discrete fracture network	Determistic continum mode	Deterministic discrete fracture network model.	Stochastic Discrete Fracture Network (DFN) Model	Porous medium, dual porosity	Stochastic continuum model	Continuum model based on a fracture network.
Process description	Advection	Advection and diffusion, spreading due to spatially variable velocity and molecular diffusion.	Advection and diffusion. Spreading due to both longitudinal dispersion in channels and to complete mixing at channel intersections.	Advection Dispersion Diffusion	Advection and dispersion	Advection Dispersion Molecular diffusion	Tasks 1 and 2: Advection corrected for fluid density. Task 3: Advection with stochastic dispersion along flow lines.	Advection, dispersion, molecular and matrix diffusion	Advection and diffusion, spreading due to spatially variable velocity and molecular diffusion.	Advection, spreading due to spatially variable velocities in the fracture network.
Geometric framework and parameters	Model size : size of the M3 model : 3.750x 2620x1500 km^3 Local fractures : Most of the deterministic local features, only EW-7 and NNW-3 are not represented. Regional fractures : SFZ-03, SFZ-04, SFZ-05, SFZ-07 (continuation of EW-1), SFZ-11, SFZ-12 (continuation of NE-1), SFZ-14 Rock Mass Domain : deterministic. Two domains : SRD-4 is modelled	Same as for flow problem: Deterministic features: kept 16 : EW1S, EW3, EW7, NE1, NE2, NE3, NE4N, NE4S, NNW1, NNW2, NNW3, NNW4, NNW5, NNW6, NNW7, SFZ11. Rock outside the deterministic features is not modelled	Model boundaries, in Aspo coordinates: X = 1000 to 3000 Y = 6000 to 8000 Z = -1000 to 0 Deterministic features: the 21 fracture zones as given in the data set Rock outside fracture zones not modelled	2 x 1.8 x 1 km^3 A selection of 10 deterministic features provided in the data set (NE-1, NE-2, NE-3, NE-4, NNW-2, NNW-4, NNW-7, EW-1 78°, EW-1 88°, EW-3) Rock domain ignored between deterministic fractures	Model size: 2.0x2.5x1 km^3 . Easting 1000-3000m, Northing 5500-8000m, 0 - -1000m in depth at Aspo coodinate Determistic features: All except for ???, which Rock outside the deterministic features modelled as determistic continuum.	Model size: 2 x 2x 1 km^3 . Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features: neglected	Model Size: N-S 2.0 km; E-W 2km; depth 1 km Deterministic features: All SKB deterministic features provided in the data set. In addition an additional “mystery feature” was added to match the drawdown responses. NNW-5 was extended north to collect more glacial water. Deterministic BH features: features added through BH sections to	Model size: cross-section hexahedron with diameter about 3.3 km, depth 1.5 km Fracture zones provided in SKB TR 97-06 Rock between the fracture zones Both the fracture zones and the rock between them modelled as dual porosity medium	Model size: 1.8x1.8x1 km^3. Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features modelled as stochastic continuum.	Model size: 1.8 x 1.8 x i km^3 Deterministic features: All deterministic features provided in the data set. Rock outside the deterministic features modelled as continuum, based on a fracture network.

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera (1)	SKB/CFE/Intera (2)
	independently						improve connectivity BH to DFN model. Stochastic features: Background features modelled using stochastic discrete features.			
Material properties	Cinematic porosity (ne)	Flow porosity (ne)	Porosity (n), dispersivity (d)	Porosity Longitudinal and transverse dispersion Diffusion Tortuosity	Flow prosity (ne) calculated from the experimetal relationship between hydraulic permeability and flow prosity. cf. Eq(8-8), pp.399, TR97-06.	Flow porosity Dispersivity Molecular diffusion coefficients	Transport aperture	Diffusion porosity (ϕ_d), fracture spacing (*2a*), matrix porosity (ϕ'), longitudinal ($\square_L$) and transversal ($\square_T$) dispersion lengths	Kinematic porosity	Kinematic porosity
Spatial assignment method	Ne based on hydraulic conductivity (TR 97-06) for each fracture, SRD4 and rock mass domain	ne based on hydraulic conductivity value (TR 97-06) for each cell in model	n based on hydraulic conductivity value (TR 97-06) for all fractures d constant in model, from TR97-06.	Deterministic values for all features	Flow prosity (ne) calculated from the experimetal relationship between hydraulic permeability and flow prosity. cf. Eq(8-8), pp.399, TR97-06 for each element.	Deterministic based in the availble data set	Aperture A = $2T^{0.5}$.	Properties given for each element in the model Depth dependent fracture spacing Kinematic porosity (ϕ_f) calculated from the hydraulic conductivity/transmissivity and the fracture spacing	Kinematic porosity based on hydraulic conductivity value (TR 97-06) for each cell in model, including deterministic features and rock outside these features.	Kinematic porosity, based on the porosities assigned to the fractures in the network.
Boundary conditions	Island and continent : 100% Meteoric water Sea : 100% Baltic water Other boundaries : Mixing ratios for endmembers based on M3 calculations	Mixing ratios for endmembers as provided as initial conditions in data sets	End member simulation: mixing ratios as provided in the data base. For the top boundary, use pure Meteoric under land and pure Baltic under sea.	Mixing ratios for reference waters derived and interpolated for discrete fractures as provided as initial conditions in data sets.	Mixing ratios for endmembers as provided as initial conditions in data sets.	Prescribed concentrations for end memebers, chlorides and 18-O, as provided in the data set for the initial conditions	Stage 1 and 2 : Initial geochemical conditions were provided at 98 locations, in Appendix 14 of Data Delivery 7 using M3. These	Land, sea, vertical edges and bottom: concentration for endmembers on the basis of the mixing ratios as provided by M3 and the inverse modelling	Initial conditions calculated as Steady State Solution. Top: 100% Meteoric on land, 100% Baltic below the Baltic Sea. Vertical and	Initial conditions calculated as Steady State Solution. Top: 100% Meteoric on land, 100% Baltic below the Baltic Sea. Vertical and

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera (1)	SKB/CFE/Intera (2)
							values were extrapolated by SKB (Rhén, 1998) using Kriging to a grid of 1000 locations. Stage 3: Chemistry at monitoring locations extrapolated to LSFs within 50m. Chemistry on LSF derived based on monitoring points, proximity to Baltic, chemical depth profiles. All particles projected to nearest LSF prior to interpolation of chemistry.	Concentration for endmembers initially also in the interior nodes based on the mixing ratios as provided by M3 and the inverse modelling, released in the first time step	botttom: Mixing ratios from assumptions and calibration. Bottom condition assumed 100% Äspö Brine.	botttom: Mixing ratios from assumptions and calibration. Bottom condition assumed Mixed water conditions.
Numerical tool	TAFFETAS	CASTEM2000	3FLO	DURST / Rockflow	FEGM/**FERM**	TRANMEF-3	FracMan / PAWorks	FEFTRA	PHOENICS	PHOENICS
Numerical method	Mixte Hybrid Finite Element	Transport of 4 concentration fields	Particle tracking method	Finite element method	Finite element method with upwinding method called Petrov-Galerkin method	Finite Elements Method	Stage 1 and 2: Graph theory searches through the channel network model. Stage 3: Particle tracking using 76 time varying head solutions.	Finite element method, the previously simulated residual pressure and concentration fields used	Solving the advection / diffusion equation for each component. Backtracking, using particle tracking, for analysis of flow paths.	Solving the advection / diffusion equation for each component. Backtracking, using particle tracking, for analysis of flow paths.
Output parameters	Concentration fields, breakthrough curves	Concentration fields and breakthrough curves	Breakthrough curves, and concentration maps.	Concentrations of reference waters	Concentration	Concentrations and mass flows	Location of particles at 30 day intervals.	Concentration	Mixing ratios for all points at all times.	Mixing ratios for all points at all times.

Summary of the models for chemical reactions calculations

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
Type of model		No chemical reaction was modelled	Principal component method.	Equilibrium and Batch Calculations	Equilibrium geochemical reaction	Transient groundwater flow and reactive transport model in a single fracture zone.	Stage 1 and 2 : Mixing using M3 chemistry Stage 3 : Principal Component Analysis (PCA)	Inverse-modelling approach	M3 (Mixing and Massbalance Modell) and Voxel 3D interpolation
Process description	Mixing : this is no chemical reactions. We performed only advection transport of the four endmemders. The model is already described in Table 1 and Table 2.		Full mixing in each cell (here each pipe) of the model. Interaction by transport of species using particle tracking method. Reactions modelled: Calcite dissolution/precipitation, plus precipitation/dissolution of carbonates, to magnesium carbonates and to gypsum	Mixing processes of different water distributions at the control points Equilibrium calculations	Mixing. Reaction: 1) HCO3 production caused by organic decomposition 2)Reduction(deoxidation) caused by Prrite dissolution 3)Calcite dissolution and sedimentation 4)Caution exchange for clay minerals 5)oxidation-reduction for HS^- /$SO4^{2-}$	Groundwater flow neglecting density effects Advection+dispersion+diffusion Homogeneous and heterogeneous chemical reactions assuming local equilibrium	Stage 1 and 2: Mixing. Stage 3: Mixing – deviation indicates chemical reactions.	Stepwise mixing calculations based on conservative Cl and ^{18}O. Reactions: Dissolution/precipitation of calcite, consumption of organic matter (CH_2O), dissolution of goethite, precipitation of pyrite, and in detail undefined ion exchange processes among pairs Na-Ca, Na-Mg and Na-Fe.	Construction of an ideal mixing model for the site based on measured groundwater composition. Calculated deviations from the ideal model for the constituents is used as an indicator of reactions. The data was used as background information for other modelling teams within TASK#5 and for M3 predictions and reporting.
Geometric framework and parameters			Coupled transport/chemistry runs in only a part of the domain of interest: main conductors upstream of Control Point number 4.	Modelling chemical equilibrium at specific control points and in fractures Identifying chemical environmental parameters by equilibrium calculations for each time step at each node (batch reactions)		Modelling groundwater flow and reactive solute transport in a single fracture zone: The Redox Zone		The reaction flow paths considered are hypothetical in the sense that no physical path between the interrelated samples was required. The aim is to describe the general evolution of water in the bedrock. It is assumed that if there would be stepwise data available along	Modelling transport and reactions at the whole site. Modelling mixing proportions in fracture network that is fairly conductive.

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
								all physical flow paths related to the chosen samples, we would find analogous chemical evolution of groundwater as described with hypothetical flow paths.	
Reaction parameters			From the Chemval data base	PH, Eh, T		Standard thermodynamics database for equilibrium constants Available and published data for cation exchange reactions Available database of the Äspö HRL for groundwater flow and transport		Detailed thermodynamic rationality or reaction rates are not taken into account but reactions take place irreversibly in one step. Modelling produces quantitative reaction amounts for predefined phases that are required to reproduce the final water composition from the defined initial water samples.	Effects from major reactions such as organic decomposition, organic redox reactions, inorganic reactions such as sulphide oxidation, dissolution and precipitation of calcite, ion exchange and sulphate reduction.
Spatial distribution of reactions assumed			Initial spatial distribution from initial conditions provided (species concentrations interpolated from grid). Later spatial distribution governed by the transport process.			All the assumed reactions could take place in the whole domain (hydrochemical system)		The *altered* meteoric reference (HAS05/-56m) has been modified in the sedimentary cover and upper parts of bedrock. Following reactions are still expected in meteoric mixing: consumption of organic matter (close to ground level we still have organic matter	Whole site

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
								available), moderate or strong precipitation of calcite (meteoric reference is high in HCO_3) and small overall mole-transfers among other dissolved ions are expected. If the *fresh* seawater dominates mixing, strong consumption of organic matter, dissolution of calcite, dissolution of Ca and Fe from CaX_2 and FeX_2/goethite, precipitation of Na and Mg to NaX and MgX_2, and precipitation of pyrite are expected. The saline reference water is well equilibrated with its environment. Only small organic matter consumption (restricted microbial activity at depth) and small overall mole-transfers among other dissolved ions are expected.	
Boundary/initial conditions for the reactions			Initial conditions: see above. Boundary conditions: fixed concentrations according to initial concentrations at		Calculated mixing portion from FEGM/FERM	Fresh water is assumed to be oxidant.	The measured chemical components at the monitoring locations.	Inverse-modelling approach is based on an attempt to understand the geochemical system along a flow path. Calculations	Calculated in relation to the selected reference waters

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
			boundary pipes. Also, pipes in contact with the atmosphere (island ground surface) are opened to CO_2 (g)					continue until acceptable set of initial water samples and reactions are found for certain final water. A previous successful (assumed steady-state) step leads to the following step, which is to find new sets of initial water samples for previous initial water samples now considered as final water samples, and so on. Steps are ultimately extended to the reference water types and then mixing fractions of the reference water types in each sample, considered in the calculation chain, can be solved.	
Numerical tool			3FLO	Phreeqc	Phreeque HARPHRQ, cf P.L. Brown et al.:HARPHRQ, UKAEA NSS/R188 (1991) HATCHES database NEA Release, cf. J.E. Cross et al.:HATCHES NSS/R212(1990)	VISUAL CORE^{2D}	Chemometric algorithm of Cave and Harmon, 1997/Cave and Wragg, 1997.	PHREEQC-2	M3
Numerical method			Principal components method. Reduce the system to be solved to *n* independent mole			Finite Elements Method for groundwater flow and transport Finite Differences	PCA	*Iterative approach* aiming to contemporaneous solution of: a) mole-balance	Multivariate statistics

TOPIC	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BGR/BMWi	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
			balance equations (Gibb's law) and *n* components. Concentrations of the principal components (e.g. Fe^{3+}, Ca^{2+}, CO_3^{2-}…) are computed after substituting each of the secondary species mass laws into the mole balance equations			Method for geochemical reactions Sequential iteration approach for coupling solute transport and chemical reactions		equations for each element or element redox state, alkalinity, and electrons b) charge balance equation c) an equation that relates the uncertainty terms for pH, alkalinity, and total dissolved inorganic carbon d) inequality constraints on the size of the uncertainty terms	
Output parameters			Concentrations of dissolved and solid-phase species, pH, in each pipe.	Element concentrations in molarities pH pe species distribution saturation indices	Amount of geochemical spices	Heads, flow, concentrations in the liquid phase, concentrations in the solid phase, pH, eH and saturation index of the minerals.	Principal components and their distribution.	Mixing proportions of reference water types for each sample involved in the calculations. Estimations of mole-transfers required reaching the final water composition in question.	Mixing proportions and deviations (used for chemical massbalance calculations) for sampling points and mixing proportions within the modelled volume.

Appendix 4: Task 5 questionnaire

(The complete answers from the modelling groups)

Compilation of answers to questionnaire concerning Task 5

Question	**ANDRA/ANTEA**	**ANDRA/CEA**	**ANDRA/ITASCA**	**BMWi/BGR**	**CRIEPI**	**ENRESA/UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/Intera**
1. SCOPE AND ISSUES									
a What was the purpose for your participation in Task 5?		Test our code and modelling capacities on a real test case with a good data base.	To gain experience on modelling for a real site, and a first limited approach to coupling of transport and geochemistry.	Validate the numerical tool that was used for flow and transport simulations; further development of this tool with respect to chemical and density effects Similar to the objectives set up for Task 5: use and integration of hydrochemical data; application of a chemical model simultaneous to hydrological computations with the aim of finally coupling different models; achieve consistency of the models Furthermore, the purpose was to demonstrate the possibility of calculating transport processes with a large scale 3-dimensional hydraulic mode, and	Our purposes for participation in Task 5 are to understand the site scale groundwater flow and solute transport. to enhance the applicability of FEGM/FERM.	The main motivation of ENRESA participation in TF5 through UDC group was the “validation” of current numerical models for coupled groundwater flow and reactive transport. Though not entirely coincident with the objectives of TF5, UDC aims were closely related to the issue of consistency of hydrodynamic and hydrogeochemical models. A strong way to check the consistency of hydrodynamic and hydrogeochemical models consists on constructing coupled flow and reactive transport models.	The JNC/Golder team undertook the DFN pipe network modelling. The overall purpose of our involvement was to use the Äspö site as an example of a generic repository location. The lessons learned, in terms of the usefulness of groundwater chemistry data, will be used to constrain future flow models and in developing an approach for optimal use of groundwater chemistry.	The purpose was to integrate the hydrodynamic model with two chemical models (M3 and inverse modelling) and to predict the conditions at Äspö.	As we performed the task for SKB, the objectives conform exactly with the ones stated in the Task #5 description.

Question	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BMWi/BGR	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
				to identify flow paths and flow velocities considering chemical components and possible reactions. In this way - knowing the permeability distribution - the expansion of radioactive substances to the biosphere after the backfilling of a future repository is possible. The Äspö HRL serves as a modelling example for the procedure.					
b What issues did you wish to address through participation in Task 5?		Flow and transport within a fractured network. Non uniqueness of the solutions for the calibration. Importance of density effects at the site. Importance of transport data with natural tracers and consistency with the different tests done.	How can geochemistry help the hydrogeological modelling? What kind of complexities are added by looking at geochemistry and hydrogeology at the same time?	Assess the extent of influence of chemical reactions on the groundwater chemistry at Äspö (granitic environment)	The accuracy of the modelling results, how to understand the site scale groundwater flow and solute transport and how to calibrate		Issues of interest included relevance of groundwater chemistry data in constraining the flow model and to develop an approach to optimise the use of groundwater chemistry. Other issues include the relevance of data for setting up a regional scale model, importance of LSFs relative to background fractures on different scales, and the effect of the fracture intersection zones.	The comparison of two chemical models: M3 and the inverse modelling.	See 1a); applies also to issues.
2. CONCEPTUAL MODEL AND DATA BASE									
a Please			See tables 1-3	See tables 1 to 3		See tables 1-3	Attached.		

Question	**ANDRA/ANTEA**	**ANDRA/CEA**	**ANDRA/ITASCA**	**BMWi/BGR**	**CRIEPI**	**ENRESA/UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/Intera**
describe your models using the tables 1-3 in the appendix.									
b To what extent have you used the data sets delivered? Please fill in Table 4 in the appendix.			See table 4	See table 4		See Table 4	Attached.		
c Specify more exactly what data in the data sets you actually used? Please fill in "Comments" in Table 4				See table 4		See Table 4	Attached.		
d What additional data did you use if any and what assumptions were made to fill in data not provided in the Data Distributions but required by your model? Please add in the last part of Table 4.			N/A	See table 4		See Table 4	Added to table.		2a)-2d), see Tables 1-4.
e Which processes are the most significant for the situation at the Äspö site during the simulation period?		Hydraulic consequences of the excavation of the tunnel.	The situation is obviously dominated by the drawdown due to the tunnel advance. Transport seems to be dominant over geochemical reactions.	The changes in the flow pattern due to the excavation of the tunnel are the most important processes for the simulation period and have to be considered. The resulting drawdown controls the mixing processes as well as	Tunnel construction and tunnel pass the hydraulic conductor domains	Groundwater flow induced by the tunnel construction, mass transfer due to advection and dispersion. These processes induce mixing of the different initial and boundary water types.	Connectivity – Modification to NNW-5, to extending it towards the north to collect glacial water. Accurate representation of LSF connectivity (required addition of a 'mystery feature') was needed to replicate the advective flow system. This is important to obtain reasonable flow pathways and velocities. Transmissivity modification	Advection and hydrodynamic dispersion. Coupled flow and transport by variable density and Darcy velocity.	Hydrology: The excavation of the tunnel changes the flow, pressure and salinity distributions significantly (upconing, lowering of groundwater

Question	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BMWi/BGR	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
				the flow velocities and flow direction. From the chemical point of view, the abundance of oxygen contained in the inflowing surface water also has a great influence on the dominant chemical reactions and existing species.			beneath Baltic to replicate the effect of lower permeability deposits on the seabed. This was required to replicate the magnitude of the drawdown at the tunnels. Advective flow – dominates over the chemical reactions. Storativity – required to obtain reasonable chemistry predictions.		table, etc.) and is hence the most important factor during the simulation period. Hydrochemistry: The changes in groundwater composition due to changes in mixing proportions.
3. MODEL GEOMETRY/STRUCTURAL MODEL									
a How did you geometrically represent the ÄSPÖ site and its features/zones?		All features are 3D, we started from 2D fractures from an automatic mesh generator (IDEAS). Finally fracture intersections are not represented but accounted for by means of continuity relations.	The fracture zones were represented as planes, bounded either by the model boundaries or by planar boundaries as specified in the data base. The “matrix” in between was not represented. In each fracture plane, flow and transport occurred along “channel pipes”, i.e. a regular grid of one-dimensionnal elements. The grid had	The Äspö site is represented by a number of deterministic fracture zones that were treated as two-dimensional planes cropping out at the surface; the rock matrix (rock mass domains) between the hydraulic features was ignored	Modelling area was represented by hex element and tunnel was represented by line elements. The hydraulic conductor domains were represented using Smeared Fracture Model; the material properties intersected by hydraulic conductors are assigned as volumetric averaging value. The topology of ÄSPÖ is neglected, but	The modelled domain was represented as a volume of 2 x 2 x 1 km. The selected modelling approach was a deterministic discrete fracture network including the main Hydraulic Conductor Domains. Our numerical models assume that the Rock Mass Domains play a much less relevant role than hydraulic-conducting domains. Therefore, they could be ignored. The comparison of measurements and model results confirm for the most part the plausibility of this assumption.	Region 2 km square by 1 km deep. The Baltic Sea and Äspö Island were treated differently in terms of applied boundary condition. All LSFs were explicitly represented as distinct discrete fractures. Background fractures were explicitly represented using a stochastic generation. Additional ‘mystery’ feature added.	Fracture zones are represented as combined quadrilaterals (see Appendix A in the reports). In the finite element mesh the fracture zones are described with 2D elements and the rock between them with 3D elements.	A model size of 1.8 x 1.8 x 1.0 km^3 was chosen. The top of the grid follows the topography. Conductivity and porosity fields were generated from a fracture network. Deterministic fracture zones were represented as planar features with a given transmissivity.

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			channels intersecting each other in four directions, at 45° angles.		the area of ÄSPÖ is modelled as the rainfall of groundwater flow. The accuracy of representation depends on spatial discrimination by finite element.				
b Which features were considered the most significant for the understanding of flow and transport in the ÄSPÖ site, and why?		NE1, NE3 and NNW4 played a dominant role in the flow calibration.	Fracture zones are the obvious key element of this flow system. They can explain most of the flow coming to the tunnel.	The selected discrete fracture zones (specified in Table 1) were considered to be the most important ones. On the one hand, they show the highest transmissivities or inflow rates to the tunnel respectively that justify their importance in the dynamic system. On the other hand, they are representative of the regional fracture system, they are located in the central area of the HRL, and extend to several hundred metres. For this reason, fractures are also included that are not intersected by the tunnel.	Hydraulic conductors defined by SR97 were considered in modelling. These fracture zones are important to evaluate groundwater flow and solute transport. In this modelling we focus on comparing measured with calculated, so it is not well understand which feature is most significant from the view of site scale groundwater flow and solute transport. But from the view	Almost all the Hydraulic Conductor Domains are important for adequately representing groundwater flow and solute transport of solutes. Only Hydraulic Conductor Domain SFZ14 is considered to have much less importance, because it is intersected neither by the tunnel nor by other Conductor Domains. Definition of proper initial and boundary conditions (especially for solute transport) was found to be also a key issue in understanding flow and transport.	The modelling indicated that the chemistry measured at the monitoring locations was dominated by the closest LSFs. Therefore, all LSFs were important. Additionally, the chemistry indicated that feature NNW-5 should be extended towards the north, to increase the proportion of glacially rich groundwater. In order to generate the correct drawdown responses an additional mystery feature was needed (in reality this may not be a single feature but a fracture zone of higher transmissivity features). This is considered important as it highlighted the need for the hydrogeological model to be both geology and hydrogeologically based.	The fracture zones NNW-2 and EW-1S seem to be important as regards to the upconing of saline water.	The major deterministic fracture zones were found to govern the drawdown calculations (in the calibration process).

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					of comparing between measured and calculated, the transmissivity of NNW-7 is the most sensitive to the calculated drawdowns.				
c Motivate selected numerical discretization in relation to used values of correlation length and/or dispersion length.		Little freedom exists for the meshing, time steps had to be adjusted. In the vicinity of the tunnel and because of the importance of the velocities, precision is not optimal.	Used 50 to 70 m grid cell size, i.e. we consider that mixing and transport tortuosity occur at this scale.	The stability and available time for the calculations were decisive for the numerical discretization. The used values for dispersion were defined considering the element dimensions.		The main constrain for numerical spatial discretization was motivated by Peclet and Courant numbers, the latter depending also on time discretization. The average size of the elements was between 20 and 40 m. Therefore, flow parameters obtained by from 30 m length packer tests were considered the most appropriate for assigning model parameters.	The FracMan DFN model did not explicitly include dispersion length – dispersion was a function of the differing tortuous pathways generated by the DFN background fractures. However, the minimum fracture size modelled effectively controls dispersion through the fracturing intensity.	The dispersivity is somewhat high in relation to the test scale, judging from Fig. 8-31 in SKB TR 97-06, where the longitudinal dispersivity (m) versus test scale (m) is presented.	The grid was made as fine as possible; the gridspacing used was 20 metres. The dispersion coefficient for salt was assumed to represent "subgrid effects" and was hence made proportional to the grid spacing. The correlation length in the conductivity and porosity fields are not related to the grid as these are generated from a fracture network.
4a. MATERIAL PROPERTIES - HYDROGEOLOGY									
a How did you		Constant for	The fracture	The distribution of	The material	Properties of Hydraulic	The material properties	The material properties are	All material

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represent the material properties in the hydraulic units used to represent the ÄSPÖ SITE?		each conductor domain. Grouting values affected are constant per conductor domain. Storage coefficients constant.	zone conductivity is integrated in the channels, with channel conductivities such that the "macro conductivity" is respected. Channel sections are computed to reproduce the actual volume available for flow, taking fracture zone porosity and width into account.	the material properties depends on the fracture zones involved. For the most part, the parameters were assigned to the features as a constant value (T, porosity); a few material properties differ from fracture to fracture (width) and have the potential to control characteristic fracture behaviour, e.g. the flow rates to the tunnel.	properties are divided into two categories. One is rock mass domain called HRD, the others are hydraulic conductor domain called HCD. Spatial distribution and deep-dependency of hydraulic permeability were neglect for HRD, and variation of hydraulic transmissivity for HCD were neglect.	Conductor Domains are assumed to be deterministic and constant throughout each domain. Each domain may have different properties (T, S, posorosity, dispersivity). Rock Mass Domains were disregarded.	considered were the transmissivity (T), size, orientation, spacing model, storativity (S) and transport aperture (A) of the fractures. Large scale and background fractures were explicitly modelled, with the porosity of the matrix being assumed negligible for advective flow, hence these parameters defined our model.	given in the elements of the hydraulic units. Values are given for each fracture zone and for the site scale rock mass domains (SRD) (inverse modelling-based hydraulic simulations) and the rock mass outside them.	properties are due to the fractures in the fracture network, except for a thin layer close to ground, for which conductivities were found in the calibration process.
b What is the basis for your assumptions regarding material properties?		Used data provided in Rhen reports.	Most properties taken from data provided. One further assumption is the 0.01 skin factor at the bottom of the Baltic. This proved necessary during model fitting to limit the inflow of Baltic water.	Material properties are strongly dependent on local conditions that can be observed by a wide scattering of the property parameters in the literature; the varying parameters were taken into consideration to estimate an order of magnitude of the parameter involved which can then be included in the model. Rock matrix can be ignored.	It is difficult and complex to consider the spatial distribution and variation of hydraulic permeability. Not considered property of unsaturated flow	Flow rates into tunnel sections not intersected by Hydraulic Conductor Domains are generally small. The width of the Hydraulic Conductor Domains, as well as the short time-scale of the model allow us to assume that the role of the rock domains in terms of flow and matrix diffusion is not relevant.	The material properties for the LSF were mainly taken from Rhén et al (1997). Storativity and aperture were assumed based on tracer and interference testing at other sites. The properties of the background fractures were stochastically derived from analysis of measured fracture data.	Homogeneous and isotropic conductivity *K* and transmissivity *T* (SKB TR 97-06). Depth dependent transmissivity for the fracture zone EW-3 (SKB TR 97-06). Widths of the fracture zones, storage coefficients *S*, specific storage S_S and the fracture spacings at the surface $2a_0$ judged from SKB TR 97-06. The longitudinal ($\square_L$) and transversal ($\square_T$) dispersion lengths are adjusted in the calibration process. An assumption is made on the depth dependence of the spacing of the water-bearing fractures based on the	Deterministic fracture zones were given transmissivities from field data. Other fractures and zones were assumed to have a transmissivity proportional to their linear size (see report for details). The transport aperture was assumed to be proportional to transmissivity. With transport

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								estimations of the size of matrix blocks: $2a = 2a_0 2^{-\frac{z}{500}}$. In the dual porosity approach the flow porosity ϕ_f is defined as the volume of fractures per unit volume of the entire rock: $\phi_f = \frac{b}{a+b}$, where experimentally $2b = 10(\frac{12\mu}{\rho_0 g}K2a)^{1/3}$. The matrix porosity is based on the measured porosity of rock samples from the Äspö HRL (SKB TR 97-06). In the inverse modelling-based hydrologic simulations in attempt to adjust the mixing proportions in the control points, depth dependent transmissivities were also given for the zones SFZ05, SFZ12 (including NE-1) and NNW-8. Somewhat more based on the measured transmissivities a depth dependence was also given for the transmissivities of the surface parts of the fracture zones in the land areas down to 200 metres to calibrate the mixing proportions of meteoric water in the control points.	aperture and thickness of a fracture given, the kinematic porosity was estimated.
c Which assumptions were the most significant, and why?				Almost all fractures are represented by the same material properties; all fractures are comparable;	Neglecting some conductive fractures in the rock mass domain	Neglecting Rock Domains resulted in substantial savings of CPU time and hardware (memory) requirements what allowed us to	The most significant assumptions relate to aperture and storativity. These are the most difficult to predict prior to chemistry data coming available.	The need to increase the dispersion lengths reflects the deficiencies of the model, but was appreciated to adjust the model due to lack of resources.	The assumptions regarding the kinematic porosity are crucial as they

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				variations of parameter values in one fracture are limited to local areas; the variation of parameter values can for the most part be compensated by an averaged value. Ignoring the rock mass domains may have an influence on the storage capacity; the drawdown simulated in the fractures is too fast in some cases and has to be controlled with recharge rates.	This neglecting will be important at high drawdown part.	simulate both transient flow and transport. The calibrated flow model reproduces accurately the natural responses of the system in terms of flow rates and groundwater heads. However, the numerical model has a tendency to slightly under-predict the flow rate and over-predict drawdowns (in almost all the control points). These discrepancies are attributed to the assumption of neglecting Rock Mass Domains.			determine the transport velocity.
4b. CHEMICAL REACTIONS - HYDROCHEMISTRY									
a What chemical reactions did you include?		No chemistry !	None in a first phase. Then, in a second phase, Calcite dissolution/precipitation, plus precipitation/dissolution of carbonates, to magnesium carbonates and to gypsum.	A part of the reactions suggested in the paper of M. Laaksoharju: " Groundwater reactions to consider within the Task 5 modelling" delivered with data 14 Chemical calculations are carried out independently of the regional flow and transport model; specific control points were chosen to carry	The following reactions are included, 1) HCO_3 production caused by decomposition of organic material in meteoric water 2) Consumption of dissolved oxygen in meteoric water by pyrite oxidation	No chemical processes are included in the site-scale Äspö model. The coupling among hydrogeology and hydrochemistry is been attempted at the Redox Zone. Preliminary results of a groundwater flow and reactive transport numerical model for the Redox Zone have been achieved. The numerical model accounts for aqueous complexation, acid-base, redox, mineral	Pure mixing only.	The geochemical mole-transfer reactions, considered in the inverse modelling, are dissolution/ precipitation of calcite, consumption of organic matter (CH_2O), dissolution of goethite, precipitation of pyrite, and in detail undefined ion exchange processes among pairs Na-Ca, Na-Mg and Na-Fe.	Effects from major reactions such as: organic decomposition, organic redox reactions, dissolution/precipitation of calcite, ion exchange, sulphate reduction.

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				out chemical investigations Sulphate and carbonate chemistry (diss./prec. of calcite, gypsum, dolomite, degassing of CO2(g))	3) Precipitation and dissolution of calcite 4) Cation exchange by clay minerals 5) Oxidation-reduction between HS^- and $SO4^{2-}$	dissolution-precipitation and cation exchange reactions.			
b What is the basis for your assumptions regarding the chosen chemical reactions?			We used only one type of reaction to simplify the fully coupled runs. Our objective here was to perform trial runs, not to be exhaustive.	Every chemical component was assigned one characteristic chemical reaction that explains gain or loss of this species. A comparison of calculated element concentrations following the conservative mixing model approach compared to measured element concentrations in the water samples was used to identify deviations which may be explained by chemical reactions. Available and usable data base from measurements and sampling; Al-measurements were not available thus e.g. silicate reactions could not be included	The chosen chemical reactions are based on 'Groundwater reaction to consider within the Task 5 modeling'.	Field measurements and conceptual models proposed by the Redox Zone Experiment Project (Banwart et al., 1995).	The error term for our Stage 3 chemistry modelling is a measure of the magnitude of the chemical reactions. It is believed that contributions of reactions to chemical variability is small owing to principal components attributable to reactions having small eigen values, though further work would be needed to confirm this. The M3 code derived chemistry values at the grid locations used for Stages 1 and 2 are based on mixing.	The inverse-modelling approach was simplified as much as possible. Only cation balances among ions Na, Ca, Mg and Fe were considered excluding potassium, i.e. dissolvable silicate phases were not considered. In respect HCO_3, it was assumed that the main processes producing bicarbonate are anaerobic oxidation of organic matter (CH_2O) and dissolution of calcite. The main process consuming bicarbonate is precipitation of calcite. Similarly, in the case of SO_4 it was assumed that sulphate dissolved into shallow groundwater is mostly directly or indirectly contributed from seawater. Sulphate is reduced and precipitated away only as pyrite, and pyrite oxidation is not considered as a source of aqueous sulphate.	Major reactions are the main modifiers of the groundwater composition.
c Which reactions were the most			N/A	The assessment of which reactions are the most significant	The following reactions are significant,	Cation Exchange between Na / Ca was quantitatively found out	n/a	The reactions and the amounts of reactions depend on where in the model the study point is	Biogenic reactions (i.e gain of HCO_3

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significant, and why?				depends on the identification of deviations in measured concentrations and the modelled mixing distribution. The most significant deviations occur for Ca^{2+}, Mg^{2+}, HCO_3^-, and SO_4^{2-}. The reactions looked at more closely include these components.	Decomposition of organic materia control HCO^{3-} concentration Caution exchange reactions affected the concentration of cautions	to explain the observed “excess” in Na. Exchange capacity proposed by Banwart et al (1995) must be increased in 2 orders of magnitude. Dissolution/precipitation of Redox sensitive mineral phases (pyrite, goetite). The presence of trace amounts of pyrite is enough to maintain reducing conditions (similar to those measured in the field) around the tunnel during the experiment. Calcite dissolution/precipitation. No suitable conceptual explanation exists for the dramatic increase in bicarbonate and sulphate concentrations during the Redox Experiment. Several hypothesis have been quantitatively tested by means of reactive transport numerical modelling.		located. The modelled reactions among undisturbed, well-mixed and well-equilibrated samples in the moderate depth of the Äspö model indicate that mole-transfers are in these cases small. Frequent reactions, such as dissolution/precipitation of *calcite*, precipitation of *goethite*, and Na-Mg and Na-Fe *exchanges* are small, usually clearly less than 0.5 mmol/l in a steady-state step. In many cases, mixing of well-equilibrated samples is practically conservative. With the reference waters used in the current inverse modelling, the large mixing proportions of *fresh* seawater in final water indicate considerable dissolution of organic matter and calcite, precipitation of pyrite, dissolution of Ca, Fe, and precipitation of Na, Mg. All reactions defined are vital. Anion balances (HCO_3^-, SO_4^{2-}) are adjusted with significant dissolution of calcite and organic matter, and precipitation of pyrite. Adjustments in anion concentrations require significant counterbalancing among cations to fulfil the electroneutrality and observed concentrations. The question of significant reactions is strongly related to the question: how the reference	which can indicate organic decomposition) can control the redox state of the groundwaters.

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								water types are found and/or can be defined? In the optimum case, all reference waters have equilibrated with the currently prevailing conditions in bedrock as well as possible, and at the same time they have mixed to each other as little as possible. If it would be possible to find or define reasonable average *altered* seawater the reactions considered above would be significantly smaller.	
5a. BOUNDARY CONDITIONS FOR HYDROGEOLOGICAL MODEL									
a What boundary conditions were used in the modelling of the ÄSPÖ site tests?		The ones from Svensson regional model and were kept constant throughout the tunnel progression.	See 5b	No-flow at bottom Recharge rate for Äspö Island (upper boundary) Prescribed groundwater heads of zero at vertical boundaries and for the Baltic Sea (upper boundary) Prescribed inflow rates to the tunnel (internal boundaries) For transport calculations: interpolation of grid data from M3 calculations with boundary and initial conditions;	Prescribed flux at weir in the tunnel Prescribed pressure at the top and the side of modelling area No flux at bottom of modelling area and constant flux at ÄSPÖ Prescribed concentration at the top and side boundary of modelling area were used, and the values of boundary were calculated from provided	Prescribed groundwater head equals to the initial value on the side boundaries and Baltic Sea. Prescribed recharge rate on top of the conductive features (5 mm/year at the island). Impervious boundary at the bottom.	See table 1 'boundary conditions' for details.	Salinity (M3-based simulations) or chloride (inverse modelling-based simulations) was given on the sides of the model. The residual pressure boundary condition on the vertical edges was calculated on the basis of the salinity/chloride distribution. The boundary conditions given initially in the interior nodes were released in the first time step. The residual pressure boundary condition at the bottom was also released. Groundwater table was initially applied over the Äspö island, but was replaced by a flow rate boundary condition in the second time step, when the tunnel was modelled for the first time. The residual pressure boundary condition for the flow	Top boundary: Given recharge on Äspö, fixed pressure and salinity below the Baltic Sea. Vertical and bottom boundaries: From a regional model.

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				hydrochemical conditions were assigned to the discrete fractures Vertical, upper and bottom boundaries: fixed water composition corresponding to the initial conditions	data set.			equation and the flow rate boundary condition for the transport equation were given in the tunnel and the shaft. The concentration boundary condition for the transport equation of each water type was derived from the chemical model. The boundary condition given initially in the interior nodes was released in the first time step.	
b What was the basis for your assumptions regarding boundary conditions?		Interpolation from a model based on a larger regional domain. The values were kept constant during the test.		BC must represent the regional hydraulic and chemical conditions Construct a model that represents large scale processes and focuses on the spiral tunnel as the central part of the model Usefulness of interpolated grid data for the mixing proportions Model not sensitive to boundary conditions, model border not reached; but very sensitive to initial distribution	It is difficult to quantify the skin effect of tunnel, so prescribed flux at weir of tunnel are used. Side and bottom boundaries are not influenced to the calculation result so much, so above mentioned boundaries were assumed.	The lack of data about deep and lateral side boundaries. Previous estimations about deep recharge at the Äspö site.	Base – Typical assumption for variable salinity flow with base not close to tunnel. Sides – The DFN approach provides less sensitivity to fracture intensity for constant head boundary conditions. Therefore a head, not flow, boundary condition was chosen. The values were based on the larger scale model of Svensson (1999). Baltic Sea – constant head = 0.0. Assumed good connection to the seabed. Äspö Island – differing net infiltration levels assumed. Tunnel and shafts – flow rate equal to the measured inflows into the tunnels/shafts.	The salinity or chloride boundary condition was given on the basis of the corresponding chemical model. Groundwater table applied over the Äspö island had to be replaced by a flow rate boundary condition due to the tunnel excavation. The residual pressure boundary condition in the tunnel and the shaft was fixed utilising the measured freshwater head in the nearest borehole sections. The flow rate boundary condition in the tunnel and the shaft was given on the basis of the measured flow at the weirs.	Top boundary: Estimated precipitation minus evaporation for the area. Below the Baltic Sea: "Seems correct". Vertical and bottom boundaries: Best possible estimates available.
c Which assumptions were the most significant, and why?		No sensitivity analysis was fulfilled.		Measured pressure values in boreholes can be used to estimate the lateral extension of the drawdown funnel and the maximum depth	Initial and boundary condition for solute transport The mixing portions of four end-members	Sensitivity analyses indicate that the numerical model is almost not sensitive with respect to the boundary conditions.	The model is sensitive to the tunnel inflows (set by data provided) and the boundary conditions on the model surface (i.e. Baltic and Äspö Island). The model surface was sensitive because a large	The tunnel and shaft effect was modelled by giving the above mentioned boundary conditions in the tunnel and the shaft. Thus, the assumptions concerning these boundary conditions are very important.	No sensitivity tests were performed. However, it seems important that more Meteoric

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				of the groundwater table Vertical and bottom boundaries are for the most part not reached by changes of the flow system and do not influence the central part of the model; fixed pressure and concentrations can be chosen for an influx with a constant composition	located at the upper part of the tunnel depend on boundary value, because the transport time is quit shorter than simulation time.		proportion of the inflows came from above (due to lower density fluid and the primarily sub-vertical LSFs).		water should infiltrate when the tunnel is present. The top boundary condition used, and the algorithm for the unsaturated zone, ensures this.
5b. BOUNDARY/INITIAL CONDITIONS FOR HYDROCHEMICAL MODEL									
a What boundary conditions were used in the modelling of the ÄSPÖ site tests?		The ones from M3 model (before and after excavation) for boundary conditions and initial conditions from M3 before excavation.	Top surface: constant flux under land, and constant head (with skin factor) under sea. Vertical faces: constant head Bottom face: no flux On all imposed-head boundaries, the value is set to 0. The imposed constant flux is 25mm per year on all emerged	Distribution of reference waters according to M3 grid data Element concentrations calculated from mixing proportions of reference waters resulting from the transport model Measured element concentrations at boreholes	Equibirium geochemical reactions calculated by HARPHRQ were considered for the mixing rates calculated by solute transport model, so the evaluation coupling geohydrogical and geochemical were not conducted.	Prescribed concentrations on the lateral and bottom sides, and Baltic and meteoric concentrations on the top boundary.	Stages 1 and 2 used the end members in Appendix 9 of the data deliveries. Stage 3 used the 7 principal components derived using the PCA approach and the chemometric code of Cave et al.	The water samples used for inverse calculations, were divided into two subsets (undisturbed and disturbed) in respect of the excavations of the Äspö tunnel system. The undisturbed sample set, were used for identification of the reference water types that have been active in the Äspö HRL volume, for describing the general evolution of water in the bedrock, and for defining the depth relations and distributions of reference water types in the undisturbed model volume. The depth distributions of the reference water types form the initial condition for the	Geographical locations of the reference waters.

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			lands. The total influx is distributed equally on all land nodes.					simulation exercise. At the vertical and bottom boundaries of the model these undisturbed conditions are assumed to be valid throughout the exercise. The depth distribution of chloride (cf. item 5a-a) is calculated from the depth distributions of the reference water types. The depth distribution of chloride (i.e. density) is assumed be constant within the model volume during the exercise.	
b What was the basis for your assumptions regarding boundary conditions?		Boundary conditions were chosen from M3 for consistency reasons since results are compared with M3 at control points. The data was interpolated from M3 grid.	Head boundaries chosen for simplicity. Imposed constant flux calibrated to obtain plausible heads before tunnel construction. Skin factor used to limit influx of Baltic water, based on Control Point observations.	Deviations of modelled and measured concentrations of conservative elements are negligible Conservative elements must be explained by pure mixing, e.g. dilution		Most of the chemical components show a stratified pattern under undisturbed conditions, which was the reason to assume the initial concentration as the prescribed value on the sides. The lack of data at depths greater than 1000 m was a limiting factor to choose the appropriate bottom boundary condition.	Stage 1 and 2 models used the previous SKB modelling to provide better coverage of the modelling region. The few data points available limited the chemistry resolution. Based on earlier modelling, in Stage 3 it was felt that the LSFs dominated the chemistry. Therefore Golder developed an independent scheme for extrapolating measured chemistry throughout the model. The chemistry at the measurement locations was changed from the M3 values to those derived by Cave based on the PCA approach.	It is assumed that the Quaternary history of the Äspö area is reflected in the general evolution of water in the bedrock, and in the depth distributions of reference water types.	Field observations.
c Which assumptions were the most significant, and why?		Behavior in the upper part of the model depends strongly on boundary conditions due to quick transfer times.	All of them!! In fact, as described in our report, boundary conditions govern most of the response.	Classification and element composition of reference waters according to M3 data is suitable for decribing chemical characteristics at the Äspö site Deviations of non-	Decomposition of organic material and caution exchange Because they are sensitive to the results	Sensitivity analyses results definitely indicate that the model is strongly sensitive to the initial distribution of concentrations.	One major deduction was that the chemistry below Äspö Island and the Baltic Sea was substantially different, and incorporating this into the extrapolation/interpolation scheme was critical.	The undisturbed sample set utilised in the depth distribution estimations is collected solely from the Äspö Island, though also the reference water type distributions below the sea areas are also estimated. Furthermore, it is assumed that the undisturbed depth distributions of reference water	Glacial water is a historical water type which is not reproduced and should therefore not increase during the tunnel construction.

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				conservatives compared to mixing compositions are due to reactions				types can present the areal model boundaries also during the disturbed part of the exercise. This is reasonable if the model boundaries remain undisturbed during the disturbed condition simulations and the detected local depth distribution can be extended to the areal scale. The density distribution does not change during simulations. However, inverse calculations exhibit significant drawdown of meteoric and fresh seawater, and moreover considerable up welling of saline water during the disturbed conditions.	The observations confirmed this assumption.
6. MODEL CALIBRATION									
a To what extent did you calibrate your model on the provided hydraulic information? (Steady state and transient hydraulic head etc.)		First compare model with stationary results by Svensson corresponding to situation before excavation and mean transmissivities provided. Then modify transmissivity values as well as resistance values corresponding to grouting in the tunnel. Calibration was done	Calibrated by imposing the flowrates in the tunnel and trying to reproduce available drawdown histories in boreholes.	Influx to the tunnel measured at the weirs used for assigning flow rates to specific fractures Inflow of meteoric water into the fractures at top boundaries derived from recharge rate on Äspö given in the literature Several runs to achieve correspondence with measured time series of heads and flux	The model calibration were performed for transient state using time series of drawdowns.	A great effort of calibration was made for the groundwater numerical model. Hand calibration with more than 30 runs of the transient model were performed and numerical results were compared against time series data of inflows into the tunnel and groundwater heads in the boreholes.	The heads were used to calibrate the transmissivities and connectivity of the DFN. The timing of the head drops during tunnelling, and the location of the drawdown responses, provide information on transmissivity and connectivity. Head data indicated the existence of a mystery large scale feature.	The residual pressure boundary condition in the tunnel and the shaft was fixed utilising the measured freshwater head in the nearest borehole sections. Groundwater table was replaced by the flow rate boundary condition, which adjusts the infiltration.	Groundwater table for natural conditions and drawdowns for tunnel front position 2 875 m.

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		mostly based on contributions from involved fractures to the total inflow in the different portions of the tunnel since inflows proved more sensitive than pressures in boreholes.							
b To what extent did you calibrate your model on the provided "transport data"? (Breakthrough curves etc.)		No calibration. Only elements of sensitivity analysis.	Not used	Change of concentration of the water content	No calibration	No calibration of transport parameters was done. Sensitivity runs were performed in order to evaluate the uncertainty in the initial and boundary conditions.	The transport data was used to calibrate the storativity and aperture of the fractures. Where appropriate the transmissivities could also be recalibrated if the chemistry indicated that the connectivity was poorly replicated – but at this site negligible changes were required.		The time history of the upconing.
c To what extent did you calibrate your model on the provided hydrochemical data? (Mixing ratios; density/salinity etc.)		Same answer.	Used them to calibrate skin factor at bottom of Baltic	Best fit of mixing proportions / element concentrations at control points and correspondence with time-dependent changes Change of concentration with time due to mixing processes identified by investigation of conservative species Cl and 18O	No calibration	No calibration with respect to hydrochemistry was done.	Model was calibrated to the end members.	The salinity or chloride boundary condition was given on the basis of the M3 modelling and the inverse modelling, respectively. The mixing ratios delivered from the chemical models were utilised to fix the concentration boundary condition for the transport equation of each water type.	Water composition in borehole section for natural conditions, tunnel front at 3 170 metres and completed tunnel (96-05).
d What parameters did you vary?		Elements of sensitivity to dispersivity were made and sensitivity to	Transmissivities in fracture zones, skin factor	Fracture width, permeability, recharge rate, specific storage coefficient; the number of	Transmissivity of fracture and hydraulic permeability of rock mass	Transmissivity and storativity of the conductive domains, leakage coefficients at the tunnel, transmissivity	Transmissivity of the mystery feature. Addition of an extra larger feature. Storativity of the LSFs.	Dispersion lengths, infiltration from the sea, transmissivities, the depth extension of the zone EW-1S, classification of sea and land nodes, the widths of	Transmissivities, conductivities of layers close to ground,

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		this parameter seems to be important. Sensitivity to boundary conditions (conditions before and after tunnel excavation).		fractures included in the model has been increased permanently		and storativity of the intersections between conductive domains and the value of groundwater recharge.		some fracture zones. Some attempts with the specific storage S_S, the matrix porosity ϕ' and the fracture spacing $2a$ were not reported.	kinematic porosity and water compositions at vertical and bottom boundaries.
e Which parameters were the most significant, and why?		Density effects proved important.	Both were important	Fracture width at tunnel intersection points were varied to control the influx and the recharge rate had great influences on the drawdown extension	Transmissivity of fracture	Calibrated parameters include transmissivity of the conductive domains and leakage coefficients of the tunnel. Sensitivity analyses indicate that the uncertainty in calibrated parameters is rather small.	Transmissivity and storativity.	The dispersion lengths, the infiltration from the sea and the transmissivities to adjust the concentration in the control points.	Most of the parameters are significant, but for different aspects (conductivity of layers close to ground are for example important for ground water table).
f Compare the calibrated model parameters with the initial data base - comments?		Calibrated and initial data base are rather consistent for the modelling work done. It seems a fair and reliable vision of the site is available.	Fracture zone NE2's transmissivity needed a 100-fold increase. This may mean there is another unknown conductor in this area. Otherwise, only NNW1 (divided by 10) and NNW3 (multiplied by 10) had to be modified significantly. Overall, the final model is relatively close	In the whole, the transmissivity has been changed by two orders of magnitude; locally the changes covered three orders of magnitude (+/-); other parameters were varied only in a small range and are mostly similar to the initial parameters	Most of hydraulic parameters were well defined to represent the change of drawdowns.	Comparison among the initial parameters and those calibrated with the numerical model are shown in the Appendix 1 of the report. The bigger effort of calibration was done for transmissivities of conductive features. Initially the geometric mean value was adopted for each conductive domain. Calibrated values of transmissivities are within the range of field measurements for all the conductive features except for NE-1 and NNW-7, in which the calibrated value was 2 and 3.5 times lower	The majority of material properties were similar to those of the base case. The major differences were the addition of a mystery feature, changes to NNW-5 and the increase in storativity in selected large scale fractures.	The dispersion lengths were not delivered in the initial data base. In the M3-based modelling the transmissivities were taken either from Model 96 or the calibrated model, which are reported in SKB TR 97-06. However, for the zone NNW-2 the mean minus standard deviation value T=2.1e-6 m^2/s was used. Additional transmissivity modifications were made in the inverse modelling-based simulations. The depth dependencies for the transmissivities of the fracture zones NNW-8, SFZ05 and SFZ12 (including NE-1) are perhaps not fully supported by the measurements.	Mostly minor changes. For conductivity of layers close to ground no initial data were available.

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			to the initial one.			than the minimum measured value, respectively			
7. SENSITIVITY ANALYSIS									
Identify the sensitivity in your model output to:									
a the discretization used		weak for flow but stronger for transport through dispersivity values chosen.	very small (tried with either square or "four directions" grids, with cell sizes from 40 to 80m). Results are almost identical	sensitive to irregular shaped (long, narrow) elements and elements with three edges (oscillation); uniform quadrilateral elements preferred	Time discretization is very sensitive to the result. Time step should be smaller than 15days to get the result in this calculation. The effect of spatial discretization is unknown.	Not sensitive	The model was relatively insensitive to the discretization, due to the dominance of the LSF on the model results.	not studied	The point to point comparisons of water composition were found to be sensitive to the discretisation. Using a neighbouring cell gives a different result.
b the transmissivity/hydraulic conductivity (distribution) used		Strong for main conductors NE1 and NE3, weaker for the others.			Sensitive	Water heads and flow rates into the tunnel are very sensitive to changes in T and S.	The transmissivity was important. It affected the match to the drawdowns during tunnel construction.	The changing of the transmissivities of the zones NNW-2 and EW-1S tenfold resulted in a change of at most 20 percentage units in the mixing proportions. The changing of the transmissivities of the zones NNW-2 and EW-1S to one tenth resulted in a change of at most 5 percentage units in the mixing proportions.	Different realisations of the background fracture networks were found to be significant for the point to point comparisons.
c transport parameters used		(see 6.d)	dispersivity not very influential. Dispersion in the model dominated by	After calculation of the flow velocity, the transport calculation was carried out based on the flow field. This process was executed	Not conducted	Concentrations are not very sensitive to changes in transport parameters.	The model showed a strong sensitivity to the choice of "particle tracking" algorithm used. Additionally the storativity and aperture effected breakthrough times, and were	The mixing proportions are sensitive to the dispersion lengths. The changing of the dispersion lengths tenfold throughout the model resulted in a change of tens percentage	The kinematic porosity was found to be important for the correct time history of the

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			mixing at intersections.	until the deviations of the measured heads, the amount of water and the concentration had been reduced to an acceptable amount. All three parameters were examined during the calculation process. Therefore, the flow field was controlled several times before the transport was calculated and was compared with the hydraulic parameters After each iteration process 3-4 fracture zones were added to the fracture network. At first, the most dominant fracture with respect to the hydraulic conditions was examined. At present, 10 fractures have been examined which are connected with each other. The 14-fracture model is ongoing. The concentration of the four waters was controlled by the amounts and flow velocity. Each water has a single meaning during the iteration process.			hard to estimate prior to the chemistry calibration.	units in the mixing proportions.	upconing.
d chemical mixing		(not studied)	full mixing: chemical	Sensitive with regard to initial -	Not conducted	Computed mixing fractions are most	Insensitive, provided the pathways/particles accounted	The mixing proportions for most studied undisturbed	To test the feasibility and

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parameters used			species are transported, then chemistry is equilibrated in every pipe, at each time step	interpolated - distribution of mixing fractions Disagreement of mixing fractions and conservative element concentrations		sensitive to initial values.	for flow weighting.	samples are results of several inverse calculation steps, and the error limits gradually get wider during each step in the calculation chain. In the case of the disturbed calibration section control points both the geochemical estimations (calculations utilise undisturbed data) and the hydrological simulations of mixing proportions (based on undisturbed depth distributions – cf. item 5b-a) have the same undisturbed geochemical data in the background. Therefore, there is no simple way to estimate the uncertainties. However, since the geochemical uncertainties for the estimations and simulations stem from the same source, it is probable that the uncertainties at least partially compensate each other. The precision of the mixing proportions is presented in the supplement report concentrating to geochemical modelling. The maximum deviations, based on assumed analytical uncertainty of the conservative parameters used (□Cl = 7%, □□^{18}O = 0.1 units), are tabulated together with the given best estimates. The addition of conservative parameters to four (Cl, Br, ^{18}O, ^{2}H), without tightening the assumed uncertainties, would greatly improve the robustness of the mixing proportion	sensitivity of the selected reference waters.

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								results. The deficiencies in the analytical data did not allow the usage of more than two conservative parameters as basis of mixing calculations.	
e chemical reaction parameters used		(not modelled)	From CHEMVAL data base		Not conducted	Reactive transport modelling at the Redox Zone indicate that computed concetrations are sensitive to transport parameters (dispersivity, porosity) and chemical parameters such as exchange capacity for the clayely fracture fillings.	Stage 3 model used the error term to measure the importance of the chemical reactions.	The geochemical reactions are supposed to have no role to the sensitivity of the hydrological simulations. The residual pressure boundary condition is based on the estimated conservative chloride distribution, and the mixing portions transported are conservative. The geochemical mixing portion calculations are based solely on conservative parameters, and appropriate geochemical adjustments to hydrological simulation results are made in one post-simulation reaction step. The maximum deviations of mole-transfers related to phases (calcite, CH_2O, goethite, pyrite, NaX, CaX_2, MgX_2 and FeX_2) were calculated, based on the assumed analytical uncertainty of the chemical parameters (uncertainty for Na, Ca, Mg, Fe_{tot}, HCO_3 and SO_4 7%, and for pH 0.1 units) subject to mole-transfer reactions. The deviations are presented in the supplementary report.	To test the feasibility and sensitivity of the selected mixing model.
8. LESSONS LEARNED									
a Given your experience in implementing and modelling the ÄSPÖ site,									

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what changes do you recommend with regards to:									
- Experimental site characterisation?		OK		No changes	More time series of concentration at certain point	A more detailed characterization in terms of undisturbed distribution of groundwater concentrations.	Task 5 demonstrated the importance of collecting high quality, well controlled geochemical data from the very start of the project, and collecting that data on a regular basis throughout the project life. Radioisotope data would be useful in order to derive water residence time, so that we can assess the applicability of the model to natural conditions/timescales which are more relevant to PA.	In the view of inverse modelling based estimations and simulations, distinct deviations in hydrological performance measures, as well as in estimated and simulated mixing proportion results were detected. In both cases deviations seem to start as a control point turns into the disturbed condition. These difficulties raised three principal questions: "are the hydrological/structural properties of the fracture zones correctly estimated at depth, are the structural relations between the fracture zones correctly defined, and is the open tunnel effect taken correctly into account in the hydrological model?"	Site characterisation: As we are dealing with a transport problem more information about the kinematic porosity is needed. More information is needed concerning chemical time series. The sampling should be simultaneously from several or all boreholes at a site only then the chemical dynamics of a site can be modelled.
- Presentation of characterisation data?		OK		No changes		OK	JNC/Golder proposed to address the capability of a model calibrated using only hydrogeological data to predict groundwater chemistry. So, data delivery of groundwater chemistry data should have been delayed. Where data delivered for the project had been pre-processed, it would have been valuable to know initially how the processing had been done (e.g. (1) to know exactly how the M3	mainly good enough this way	Presentation OK.

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							code calculated end-members (this information was provided prior to stage 3 modelling), e.g. (2) to know how data were interpolated onto the regular grid used as an initial condition). Include a legend and units for all provided information. Where feasible, provide all the relevant data in one package. Summary table of available data, and most recent version (particularly if some data exists under a different task). For time dependent data it would have been useful to know whether the chemistry recorded was likely already influenced by the effect of the tunnel drawdowns or is at its initial state.		
- Performance measures and presentation formats?		OK		No changes	More simple geochemical distribution should be simulated as performance measurement.	OK	Fewer performance measures as the large number of measures became distracting. A few core measures would result in a more uniform reporting by the groups. The presentation formats could also be rationalised to fewer tables but more explicitly defined. Perhaps some of the core information could be pasted into provided tables – so that the results from the groups were more uniform. Obviously the output from DFN and EPM models are very different, so the core tables would need to be carefully defined. Perhaps we could have a few very well defined "core" or "level 1" objectives and		Performance measures: The present study indicates that point by point comparisons is not the best approach (see report). Overall similarities/differences in the site description is of greater importance and interest than accuracy of predictions at selected sampling points.

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							deliverables to be addressed by all modelling teams. Followed by a range of optional “level 2” and “level 3” objectives/deliverables each to be addressed by a few modelling teams. Tritium data were provided, but it was learnt that they should not be used in a quantitative way for distinguishing proportions of mixing components. Inclusion or exclusion of tritium data caused the results of PCA to change. Inclusion of tritium data in calculations of mixing proportions is unsound because these data were obtained over a time frame similar to the half life of tritium.		
b What additional site-specific data would be required to make a more reliable prediction of the tracer experiments?		More about dispersivity and fracture variability in regional scale conducting features. Presence of non saturated flow phenomena below Äspö ?		Analysis of additional conservative tracers in the water samples (Bromine, reliable Tritium data) Comparable time series of hydrological and hydrochemical measurements at boreholes; complete or additional analysis (Br^-, Tritium, Al, C and S isotope data), e.g. to consider additional conservative tracers or to assess incongruent hydrolysis processes	More typical distribution of solute and more time series	Data about surface recharge reaching the deep aquifer. Skin factors or leakage coefficients at the tunnel surroundings. More complete time-series for groundwater concentrations at the boreholes.	The tracer predictions would benefit from stating how the values of porosity, transport aperture, free water diffusion, etc. (if provided) were derived. Are these site specific or generic? Are these values the median of ranges, should we use a distribution of values, and how much confidence do we have in these parameters. In many cases it is difficult to find out the test specifics (i.e. how the test was actually done on site) because this information is not part of the core data delivery. This has a big effect on the boundary conditions for many of the numerical transport models. In the light of experience in other programmes it is	Considering the site scale model there may be a need of more accurate definition of hydrological/structural properties of the fracture zones.	Boundary conditions (different for all vertical boundaries) of water composition. Kinematic porosities. Better time series.

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							considered likely that trace element data, especially Br data, would improve the definition of end-members and their mixing proportions.		
c What conclusions can be made regarding your conceptual model utilised for the exercise?		It is still at a preliminary stage, and would require further calibration if time was provided. It is nevertheless sensitive to boundary and initial conditions (M3) as well as to dispersivity coefficients used.		Conceptual model is suitable for identifying and modelling significant flow and mixing processes connected to the Äspö HRL at the site scale Main processes included in considering deterministic fractures and ignoring matrix effects Reproduction of conservative mixing in terms of four reference waters is satisfactory, but must be improved by considering conservative elements like chloride Groundwater classification into different types very helpful for identification of mixing processes	The groundwater flow was well represented using aforementioned conceptual model.	The impact of the tunnel construction can be reproduced accurately by numerical modelling just accounting for the main hydraulic conductor domains. A good calibrated groundwater flow model is able to reproduce conservative concentration evolutions in most of the observation points. Evaluation of the main uncertainties of the model allows us to make reliable predictions of conservative solutes.	The DFN and DFN/CN conceptual models used by the JNC/Golder team appear to be well applicable to the site and we are generally pleased with the results of our predictions. However, this site shows a dominance of LSF responses, and less large scale channelling. The lack of channelling makes the pipe discretization less appealing than the standard DFN approach (although still a reasonable alternative approach for the smaller scale models).	It involves a large number of somewhat uncertain parameters, also due to the dual porosity approach.	The model used in stage one (called Model99 in the report) was too simple, the model of stage two is a major improvement conceptually. The introduction of MWH, MWL and MWB (see report) was very useful. For M3, the conceptual paleohydrolological model of Äspö seems to be supported by observations.
d What additional generic research results are required to improve the				Higher resolution and consideration of local differences concerning material properties and model parameters to	Paleohydrogy using stable isotope	Exploring the connectivity among the main conductive features. Field experiments to	Generally the Task 5 modelling has shown that the larger scale responses are well replicated, typically better than smaller scale tracer tests where local connectivity is harder to predict	See items 8a and b.	The descriptive model is good.

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ability to carry out predictive modelling of transport on the site scale?				implement less important features that are controlled by small scale effects In general bring together the effects identified at different scales to better represent natural conditions and optimise the model output Recharge rate and amount of infiltration at depth		evaluate the value of the recharge. A more detailed sampling program for chemical analyses. Finding out strongest hydrochemical conceptual models to explain the evolution of some groundwater components (sulfate increase induced by tunnel construction), for which there is not a satisfactory explanation.	and the sensitivity to material property heterogeneity greater. The main limitation to the current model was the uncertainty in the initial spatial distributions of chemically distinct groundwaters. Therefore, it would be beneficial to conduct additional research aimed at defining the initial chemical conditions more accurately throughout the region. An additional limitation was the separation of uncertainty in chemical predictions due to spatial uncertainty (i.e. are we correctly predicting where it came from) from that due to chemical reactions (i.e. has it chemically changed due to mixing). The PCA method used is thought to distinguish reaction-dependent components from mixing-dependent components and based on the PCA, it was assumed that reaction-dependent uncertainties were small compared to other uncertainties. However, additional research is needed to confirm or refute the validity of this assumption and to refine the PCA methodology for distinguishing reaction-dependent components. Additional research in the following fields would also be useful: A more accurate initial condition for the chemistry throughout the region. Long term injection of non-		

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							reactive tracers over a longer time frame might allow the true accuracy of the numerical models to be assessed. A method to determine transport aperture from aperture measurements in boreholes or excavations. Field testing to correlate transport aperture to transmissivity and determine whether the relationship is scale dependent. (Transport aperture has been correlated to tracer tests for specific sites).		
9. RESOLUTION OF ISSUES AND UNCERTAINTIES									
a What inferences did you make regarding the descriptive structural-hydraulic model on the site scale for the ÄSPÖ site?		All parameters for flow and transport do not vary among the fractures which are deterministically considered and taken planar.		Available data base provides an understanding of the hydrological and hydrochemical conditions and allows the development of a suitable conceptual model that accounts for the most significant processes occurring during tunnel construction Groundwater system can be reproduced including the main structural elements of the site and ignoring the rock mass domain	The location of NNW-7 could be located little bit close to KAS02	Main fracture zones strongly control the hydrogeology of the Äspö site. The great effort in structural and hydraulic characterization of the Äspö site provides a good knowledge of the hydrogeology and allows setting up a sound conceptual model, which is necessary for constructing sound numerical models. Tunnel construction produces a hydrogeological disturbance, which is the responsible of the	The structural model provided by SKB was sufficient to construct a framework for the hydrogeology of the site. The hydrogeological data was required however, to add the additional mystery feature. The additional geochemical data was required to alter the geometry of feature NNW-5, extending it northwards into a region of more glacially rich groundwater.	The inverse modelling based simulations run into several difficulties. The main reasons were interpreted to result from the problems indicated in the item 8a. In our model also several functional hydrological depth relations were assumed for the fracture zones and were not calibrated to measured values. In the case of an aerial conductive fracture zone, the physical dimensions of rock mechanically weak and the hydrologically conductive zone are perhaps frequently (?) considered as equal, though almost without exception the former has clearly larger dimensions than the latter.	The descriptive model is good.

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						occurrence of large mass transfer into the groundwater. Groundwater flow and mass transfer processes produce a mixing of waters which is responsible for the hydrochemical evolution of the Äspö site. In spite of the fact that most of the primary components can be explained by conservative transport, there are some species influenced by chemical processes. The evolution of these reactive species could strongly modify important hydrochemical conditions of the system such as pH or redox conditions.		Possibly, this happens simply because only the mechanically weak zone can be measured during the geological mapping.	
b What inference did you make regarding the active hydochemical processes, hydrochemical data provided and the hydrochemical changes calculated?		All along the line of the reports by Rhen.		The induced mixing processes can largely explain the changing chemical compositions Conservative mixing approach helps to identify deviations of reactive species Further deviations can be understood by assuming chemical reactions which are mostly due to changes in the chemical boundary conditions (pH, Eh, which in turn control reactions	The groundwater under Aspo could be replaced by Baltic water.	The main detected hydrochemical processes include pyrite dissolution, calcite dissolution/precipitation and cation exchange. There remain uncertainties about chemical processes affecting bicarbonate and sulphate evolution after the tunnel construction.	Generally the end member chemistry measured during the modelled period did not change very much. Therefore the prediction of the initial chemistry at any prediction location was important. Hence the methodology used for the chemistry extrapolation/interpolation was critical. The lack of measured changes provided a lower bound on the required storage in the fractures and matrix in the vicinity of the measurement. However, less constraint on connectivity was obtained than hoped for.	The important geochemical processes that should be taken into account in the modellings and the extent of hydrochemical changes in these processes depend strongly on the choice of the reference water types. If the meteoric water reference composition is defined according to an average precipitation, large mole-transfers can be expected to occur during infiltration through organically active Quaternary sedimentary cover and upper parts of bedrock. Similarly, if *fresh* Baltic Sea water reference could be substituted with an *altered*	Helpful in understanding the complexity of the site in terms of flow and reactions affecting the obtained groundwater composition.

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				like calcite dissolution/precipitation, pyrite dissolution, and ion exchange				Baltic Sea reference, sampled below the sea bottom sediments, significantly smaller mole-transfers could be expected than presented in the supplement geochemical report for *fresh* Baltic Sea. The choice problem in the case of saline reference is analogous to the former two reference water types and is discussed in more detail in the supplement report. There were two significant analytical deficiencies considering the hydrochemical data. The reported Br values in the data have been proven to be imprecise, and mostly useless in geochemical calculations. However, Br would be an important parameter in the mixing-proportion error reduction attempts. As well, the addition of carbon and sulphur isotopic values into the data would increase significantly the reliability of the geochemical modelling results. The processes related to Na, Ca, Mg and Fe were not defined in detail. More or less likely reacting phases, in addition to normal exchange processes, are montmorillonite, kaolinite and chlorite that are usual alteration products of feldspars and biotite. These mineral phases have not been included into inverse calculations because Al concentrations in the samples were not reported. Therefore,	

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								ion-exchange processes utilised must be considered as lumped approximations. There was deficiency of undisturbed samples available for inverse-modelling calculations, basically because ^{18}O values were not available for all analysed samples. However, the amount of variables in the inverse calculations may easily increase to 15–20 (reference water types + reacting phases) and the amount of samples should clearly exceed this number. This was an important reason as well to minimise reactions considered and use lumped phases.	
c What issues did your model application resolve?		Importance of density effects. Fairly good consistency for the Hydraulic model.		Disturbance of groundwater system as a result of tunnel construction; drawdown funnel; identification of transport processes; illustration of water distribution in the fractures; identification or exclusion of possible reactions; trend of chemical evolution	The application of calculation method is good for compiling the hydrogeological and hydrochemical information. For evaluating the geochemical distribution, more interpretations are needed to understand the groundwater flow.	The uncertainty related with the hydraulic behaviour of the intersection zones between hydraulic conductor domains is not very relevant for the hydrogeological response of the system. Mixing of water due to conservative mass transfer into the groundwater can explain the hydrochemical behaviour of the system for most of the species. Computed results based in a hydrodynamic approach are quite consistent with the	Strong and fast drawdown responses due to larger scale feature not identified by regional geological model.	Generally in the M3-based simulations, the brine water seems to remain steady, except in the prediction section, where it is mildly increasing. The glacial water decreases, because it is a relict component in the present-day groundwater conditions. In the control point KA3385A the future condition of the glacial component seems nearly unvarying. The meteoric water generally increases. In the control points SA2783A and KA3385A it remains steady in the near future, however. The overall future condition of the Baltic water seems quite steady. These results are fairly well in line with those of the M3 model.	It is technically possible to carry out a simulation like this (not a trivial task!) The integration of hydrology and chemistry as manifested in the mixing proportions of the four water types is very useful. Mixing proportions summarise the groundwater composition and offers the tool for

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						results computed with a mixing model. The hydrodynamic model results support the conclusions of mixing hydrochemical models.			integration with the hydromodel. A hydromodel can be used to predict an operational groundwater composition at any point by using the mixing proportions of the reference waters.
d What additional issues were raised by the model application?		Improve the code in the future by including 2D features within 3D problems.		Difficulties in explaining chemical development for every component at control points; deviation from general trend may be due to local conditions (e.g. grouting, pumping, in situ tests) Influence of density effects It has not been possible to calculate the groundwater lowering three dimensionally considering the two phase flow in the area of Äspö island The influence of the annual precipitation on the recharging of meteoric water is	It is difficult to calibrate the model using hydrochemical data, because the distribution of hydrochemical spices are not well known the initial and boundary condition comparing the groundwater flow. To get more effective results, selecting the hydrochemical spices that has more acceptable and distinctive features are necessary.	A coupled numerical modelling of groundwater flow, transport of solutes and geochemical reactions has been performed. An alternative conceptual model for the hydrogeology of the Redox Zone has been formulated by means of the numerical model. The coupled numerical model is able to reproduce the patterns of many chemical species. However, some discrepancies are found for bicarbonate and sulfate.	Sensitivity to assumed "initial state" chemistry throughout the region. An upper bound on the model transport apertures, and to some extent storativity, was not achieved due to the lack of variation in the measured end member chemistries. We feel that rapid chemical change mostly occurred along LSFs but not within intact rock, which is more relevant to PA.	In the inverse modelling-based simulations the hydrological model did not yield the up-coning of saline water, which is apparent on the basis of the inverse modelling results in the control points KA1755A and SA2783A. Overall, the trends in the mixing proportions calculated in the inverse model appear more clearly than in the M3 results.	Pointed to weaknesses in the continuum model used, i.e. storage of water for long time periods. The mixing portions should be used more effectively to calculate an operational turnover time for the water, and the results from the chemical modelling could be presented as flow lines for easier integration/comparison with the hydrogeological modelling.

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				dependent on the groundwater depression cone of the single fracture system associated with tunnel excavation, theses influences have not been examined sufficiently					
10. INTEGRATION OF THE HYDOGEOLOGICAL AND HYDROCHEMICAL MODELLING									
a How did you integrate the hydrogeological and hydro chemical work?		Remained at a preliminary stage due to a lack of time.	In a first phase, simply used mixing ratios to better calibrate the hydrogeological model. In a second phase, and only on a part of the domain, implemented a full transport/chemistry coupling.	Flow and transport calculations were carried out for a fracture network on a site scale considering chemical conditions by setting up a conservative mixing model using the M3 reference waters A tool was developed to perform batch reactions with PHREEQC that carries out speciation calculations for the whole fracture network resulting from the mixing model; chemical calculations carried out with PHREEQC refer to	The inconsistency between hydrogeological and hydrochemical still remain, but it may be useful to consider both on modelling.	At the site scale model (Aspo), only the consistency between hydrogeological and hydrogeochemical (mixing) models was tested by means of mixing frations. Predictions of mixing fractions derived from the hydrogeological model compared favourably with M3 results at control points. → The UDC group is the only team which has attempted a full integration of hydrogeological and hydrogeochemical models at the Redox Zone by means of a coupled flow and multicomponent reactive	The modelling steps may be summarised as: create a fracture model of the site construct flow model by adding boundary conditions and meshing the fractures calibrate to hydrogeological model data. This was done by optimising the fits to the heads measured at the monitoring sections by adapting the boundary conditions and large discrete fractures (e.g. adding a skin to the Baltic to increase modelled drawdowns, addition of "mystery feature"). following head calibration, this model was run with the initial condition groundwater chemistry and a geochemical comparison documented. the differences between the measured and modelled geochemistry were used to	They were integrated by defining the salinity/chloride and the water type boundary conditions of the hydrogeological model on the basis of the hydrochemical models. In the case of inverse-modelling approach the simulated proportions are recalculated first to the "conservative chemical compositions". These compositions are further transferred to "corrected chemical compositions" in a reaction step discussed in more detail in the geochemical supplement report.	Through the mixing portions of the four water types.

Question	ANDRA/ANTEA	ANDRA/CEA	ANDRA/ITASCA	BMWi/BGR	CRIEPI	ENRESA/UDC	JNC/GOLDER	POSIVA/VTT	SKB/CFE/Intera
				selected control points as well as to the whole fracture domain; the aim wa to identify chemical reactions that account for changes in the chemical water composition at the whole site; integration was achieved by comparing the results of the mixing model with measured element concentrations – deviations indicate possible reactions		transport model. This approach is a much stronger (and therefore more complex) way to integrate hydrogeology and hydrogeochemistry.	calibrate the hydrogeologic model. This calibration resulted in the extension of NNW-5. The integration was undertaken by decoupling the processes. The chemistry was considered as pure mixing in the particle tracking. However, a PCA methodology was used to redefine the principal components into seven types more representative of the overall chemical system.		
b How can the integration of the hydrogeological and hydrochemical work be improved?		At the point where we are, mostly by moving forth and back between both models		Develop a method for directly coupling conservative transport with a reactive transport model; changing concentrations of non-conservative elements due to reactions must have an influence on ongoing transport calculations and on the characteristics of the chemical environment		By means of a coupled flow and multicomponent reactive transport model in the way that the UDC group has done it in the Redox Zone.	Generally the most realistic independent hydrogeological and hydrochemical codes are not fully coupled. Therefore to make best use of both capabilities, the chemistry should be analysed to provide information on the mixing and location of the waters through inverse modelling. e.g. what would the chemistry have been if only advection, dispersion, and diffusion had occurred?	The calibration stage should be done more carefully. More attention should be paid to the hydraulic conductivities and the transmissivities in the upper and lower parts of the model. This could result in a better fit between the calculated and “measured” mixing proportions. In the view of inverse-modelling results, more careful definition of undisturbed condition and considerable increase of control points with time-series data would give tools for confirming structural relations, and for refining spatial hydrological and structural averages for the fracture zones.	The task #5 approach is a good one, it seems. No suggestions for improvements at this stage (wait for the evaluation of Task #5). The results of the chemical modelling should be presented as flow lines and pressure lines (if possible).
c Hydrogeologist: How has the		Mixing proportions provide	Yes, as stated above	Mixing fractions resulting from M3 approach is a helpful	To calculate the geochemical	Mixing fractions computed with M3, which contain a	The hydrochemistry provides more detailed information on the directional connectivity and	It has raised questions upon the needs and usability of hydrogeological data and thus	Pointed to the improvement of the porosity

Question	**ANDRA/ANTEA**	**ANDRA/CEA**	**ANDRA/ITASCA**	**BMWi/BGR**	**CRIEPI**	**ENRESA/UDC**	**JNC/GOLDER**	**POSIVA/VTT**	**SKB/CFE/Intera**
hydrochemistry contributed to your understanding of the hydrogeology around the Äspö site?		information about the origins and travel times for the waters. These data are nevertheless uncertain.		tool to increase the understanding of dominant processes; conservative mixing model contributes to improvement of hydrological model, but does not explain further deviations of non-conservative species	distribution is good for understanding the groundwater flow. However there are big inconsistency between measured data and calculated data.	significant uncertainty, have been found useful to shape some aspects of the flow and transport model.	aperture/storativity on a regional scale.	increased the understanding of the hydrogeology around the Äspö site.	and connectivity fields. All exchanges of matter by stagnant volumes of various types need to be considered (on a variety of time and length scales).
d Hydrochemist: How has the hydrogeology contributed to your understanding of the hydrochemistry around the Äspö site?		We stuck to mixing proportions without chemical reactions, so that flow plays a dominant role.		Only if the hydrogeology has been understood completely can assumptions be made on chemical effects; it is necessary to follow a kind of chronological order with iterative interactions		Hydrogeology has been found to be fundamental for understanding the hydrochemistry around the Äspö site	The fact that the stage 3 model produced reasonable consistency between predictions and observations improves confidence in the stage 3 model for the initial spatial distributions of chemically distinct waters. The work emphasised the importance of fracture zones for controlling mixing between chemically distinct waters and hence groundwater chemistry.	Off-focusing the detailed geochemical modelling may produce, coupled with hydrological simulations, interpretations and generalisations that may have a role in refining the site scale structural-hydrological model.	An independent model that can be used for comparison and correction of the selected chemical reference waters and conceptual model.

Appendix 5: Task 5. Properties of HCDs and HRDs

Hydraulic Conductor Domain (HCD) (a)	Proposed (b)(c)(d)(e) T (median)	Proposed (c)(d) width	ANDRA / ANTEA T	ANDRA / CEA T	ANDRA / ITASCA T	BMWi / BGR K	BMWi / BGR width	BMWi / BGR T	CRIEPI T	ENRESA / UDC K	ENRESA / UDC width	ENRESA / UDC T	JNC / GOLDER T	POSIVA / VTT T	SKB /CFE / Intera (1) T	SKB /CFE / Intera (2) T	Compared features
	(m²/s)	(m)	(m²/s)	(m²/s)	(m²/s)	(m/s)	(m)	(m²/s)	(m²/s)	(m/d)	(m)	(m²/s)	(m²/s)	(m²/s)	(m²/s)	(m²/s)	
EW-1N	1.5E-06	30			1.5E-06	5.0E-07	10.0	5.0E-06	5.2E-07	4.32E-03	30	1.5E-06	2.4E-06	5.2E-07	5.2E-07	5.2E-07	
EW-1S	2.2E-05	30		1.2E-05	2.2E-05	5.0E-07	10.0	5.0E-06	1.2E-05	9.51E-02	30	3.3E-05	3.5E-05	1.2E-05	1.2E-05	1.2E-05	
EW-1S+N			2E-05														
EW-1_perpend			1E-07														
EW-3	2.4E-05	15	2E-05	1.4E-05	3.6E-05			2.0E-06	1.7E-05	1.38E-01	15	2.4E-05	3.8E-05	1.7E-05	1.7E-05	1.7E-05	
EW-3_part						5.0E-07	5.0	2.5E-06									
EW-3_part						5.0E-07	10.0	5.0E-06									
EW-3_part						5.0E-07	0.1	5.0E-08									
EW-3_part						5.0E-07	1.0	5.0E-07									
EW-7	6.8E-05	10		1.2E-05	6.8E-05				1.5E-05	1.96E-01	10	2.3E-05	1.1E-04	1.5E-05	1.5E-05	1.5E-05	
NE-1	3.0E-04	30	3E-04	2.2E-04	4.0E-04	8.0E-07	35.0	2.8E-05	2.2E-04	1.50E-01	30	5.2E-05	4.8E-04		2.4E-04	2.4E-04	
NE-2	4.1E-07	5	1E-04	8.0E-07	4.1E-05			5.1E-06	1.2E-07	7.08E-03	5	4.1E-07	6.6E-07	1.2E-07	1.0E-06	1.0E-06	
NE-2_part						5.0E-07	10.0	5.0E-06									
NE-2_part						5.0E-07	0.1	5.0E-08									
NE-2_part						5.0E-07	1.0	5.0E-07									
NE-2_part						5.0E-07	10.0	5.0E-06									
NE-2_part						5.0E-07	30.0	1.5E-05									
NE-3	2.9E-04	50	6E-04	3.0E-04	2.9E-04	1.0E-07	35.0	3.5E-06	3.2E-04	2.72E-01	50	1.6E-04	4.6E-04	3.2E-04	3.2E-04	3.2E-04	
NE-4	3.0E-05	40	2E-04	5.6E-05	6.0E-05	5.0E-07	35.0	1.8E-05	3.1E-05			6.0E-05	4.8E-05	3.1E-05	3.1E-05	3.1E-05	
NE-4N_parall				2.5E-05	3.0E-05					6.48E-02	40	3.0E-05	2.4E-05				
NE-4N_parall				3.1E-05	3.0E-05					6.48E-02	40	3.0E-05	2.4E-05				
NW-1	1.7E-07	10	3E-07	-	1.7E-07	-	-	-	4.1E-07	1.47E-03	10	1.7E-07	2.7E-07	4.1E-07	4.1E-07	4.1E-07	
NNW-1	1.1E-05	20	1E-05	1.1E-06	1.1E-06	-	-	-	8.6E-06	3.00E-02	20	6.9E-06	1.8E-05	8.6E-06	4.0E-06	4.0E-06	
NNW-2	5.6E-05	20	4E-05	3.0E-06	3.7E-05	5.0E-07	10.0	5.0E-06	2.4E-05	2.42E-01	20	5.6E-05	9.0E-05	2.1E-06	1.2E-05	1.2E-05	
NNW-3	2.0E-05	20	-	2.0E-05	2.0E-04				2.0E-05	8.64E-02	20	2.0E-05	3.2E-05	2.0E-05	2.0E-05	2.0E-05	
NNW-4	1.5E-04	10	5E-04	1.2E-05	1.5E-04			6.1E-06	6.5E-05	2.25E-02	10	2.6E-06	2.4E-04	1.3E-05	6.5E-05	6.5E-05	
NNW-4_part						5.0E-07	20.0	1.0E-05									
NNW-4_part						5.0E-07	0.1	5.0E-08									
NNW-4_part						5.0E-07	1.0	5.0E-07									
NNW-4_part						5.0E-07	10.0	5.0E-06									
NNW-4_part						5.0E-07	30.0	1.5E-05									
NNW-5	2.0E-06	20	3E-06	4.0E-06	2.0E-06				4.0E-06	2.00E-01	20	4.6E-05	3.2E-06	4.0E-06	4.0E-06	4.0E-06	
NNW-6	1.4E-05	20	1E-05	1.4E-05	1.4E-05				1.4E-05	6.05E-02	20	1.4E-05	2.2E-05	1.4E-05	1.4E-05	1.4E-05	
NNW-7	4.8E-06	20	1E-04	5.0E-06	4.8E-06	5.0E-07	10.0	5.0E-06	1.5E-05	5.00E-03	20	1.2E-06	7.7E-06	7.5E-06	2.0E-05	2.0E-05	
NNW-8	1.0E-05	20	9E-06		1.0E-05				8.4E-06	8.64E-02	20	2.0E-05	1.6E-05	8.0E-06	8.4E-06	8.4E-06	
'Mystery feature"													1.0E-05				
SFZ01	3.0E-06	20												3.0E-06			
SFZ02	1.0E-04	20												1.0E-04			
SFZ03	3.0E-06	20	3E-06										4.8E-06	3.0E-06	3.00E-06	3.00E-06	
SFZ04	3.0E-06	20	3E-06											3.0E-06			
SFZ05	1.0E-04	20	2E-04											5.0E-04			
SFZ06	3.0E-06	20												3.0E-06			
SFZ07	3.0E-06	20	2E-05												3.00E-06	3.00E-06	
SFZ07_perpend			1E-07														
SFZ08	3.0E-06	20												3.0E-06			
SFZ09	3.0E-06	20												3.0E-06			
SFZ10	1.0E-04	20												1.0E-04			
SFZ11	3.6E-06	20	3E-06	3.6E-06	3.6E-06					1.56E-02	20	3.6E-06	5.8E-06	3.0E-06	3.00E-06	3.00E-06	
SFZ12	1.0E-04	20	3E-04											2.2E-04	1.00E-04	1.00E-04	
SFZ13	3.0E-06	20												3.0E-06			
SFZ14	3.0E-06	20	3E-06		3.6E-06								4.8E-06	3.0E-06			
SFZ14a_part					3.6E-06												
SFZ14b_part					3.6E-06												
SFZ15	1.0E-04	20												1.0E-04			

(a) : "xxxx_parall" indicates that the fracture zone has been divided into several parallell planes by the modeller. The total (added) tranmissivity for fracture zone is in row "xxxx"

"xxxx_part": indicates that the fracture zone has been divided into several parts by the modeller.The tranmissivity for fracture zone is in row "xxxx"

"xxxx_perpend": Transmissivity perpendicular to fracture zone plane

"xxxx": Transmissivity as single value or mean of "xxxx_part" or sum of "xxxx_parall"

(b) : TR 97-06, Table A2-8

(c) : TR 97-06, Table A2-7, Section 6.2.3.

(d) : TR 97-06, Table A2-6

(e) : TR 97-06, Table 6-3, Figure 6-21

Hydraulic Conductor Domain (HDR) (a)	Proposed (b) S	Proposed (b)(c) width	ANDRA / ANTEA S	ANDRA / CEA S	ANDRA / ITASCA S	BMWi / BGR Ss	BMWi / BGR width	BMWi / BGR S	CRIEPI S	ENRESA / UDC Ss	ENRESA / UDC width	ENRESA / UDC S	JNC / GOLDER S	POSIVA / VTT S	SKB /CFE / Intera (1) S (d)	SKB /CFE / Intera (2) S (d)	Compared features
	(-)	(m)	(-)	(-)	(-)	(1/m)	(m)	(-)	(-)	(1/m)	(m)	(-)	(-)	(-)	(-)	(-)	
EW-1N	2.5E-07	30		-	1.0E-06	1.0E-04	10.0	1.0E-03	3.0E-05	3.33E-06	30	1.0E-04	1.5E-06	1.0E-06			
EW-1S	2.0E-06	30		1.3E-06	2.0E-06	1.0E-04	10.0	1.0E-03	3.0E-05	4.80E-06	30	1.4E-04	1.8E-05	1.3E-06			
EW-1S+N			2.0E-06		1.0E-06												
EW-1_perpend																	
EW-3	2.2E-06	15	2.2E-06	1.4E-06	3.0E-06			4.0E-04	1.5E-05	1.03E-05	15	1.5E-04	6.2E-06	1.7E-06			
EW-3_part						1.0E-04	5.0	5.0E-04					1.9E-05				
EW-3_part						1.0E-04	10.0	1.0E-03					6.2E-06				
EW-3_part						1.0E-04	0.1	1.0E-05									
EW-3_part						1.0E-04	1.0	1.0E-04									
EW-7	4.9E-06	10	-	1.3E-06	4.9E-06	-	-	-	1.0E-05	3.50E-05	10	3.5E-04	1.0E-05	1.5E-06			
NE-1	2.6E-06	30	1.6E-05	1.2E-05	7.8E-05	1.0E-04	35.0	3.5E-03	3.0E-05	8.67E-05	30	2.6E-03	2.2E-05	-			
NE-2	8.9E-08	5	6.7E-06	1.5E-07	3.3E-06			1.0E-03	5.0E-06	2.00E-05	5	1.0E-04	2.7E-06	1.0E-06			
NE-2_part						1.0E-04	10.0	1.0E-03									
NE-2_part						1.0E-04	0.1	1.0E-05									
NE-2_part						1.0E-04	1.0	1.0E-04									
NE-2_part						1.0E-04	10.0	1.0E-03									
NE-2_part						1.0E-04	30.0	3.0E-03									
NE-3	1.5E-05	50	2.7E-05	1.6E-05	1.5E-05	1.0E-04	35.0	3.5E-03	5.0E-05	2.18E-05	50	1.1E-03	2.2E-05	1.7E-05			
NE-4	2.6E-06	40	1.2E-05	4.2E-06	4.5E-06	1.0E-04	35.0	3.5E-03	4.0E-05			2.0E-03	1.1E-05	2.7E-06			
NE-4N_parall				2.2E-06	2.6E-06					4.60E-05	40	1.8E-03	1.7E-05				
NE-4N_parall				2.7E-06	2.6E-06					4.60E-06	40	1.8E-04	4.9E-06				
NW-1	4.5E-08	10	7.0E-08	-	4.5E-08	-	-	-	1.0E-05	1.00E-05	10	1.0E-04	5.2E-07	1.0E-06			
NNW-1	5.0E-06	20	1.2E-06	1.9E-07	1.0E-04	-	-	-	2.0E-05	2.50E-06	20	5.0E-05	4.2E-06	1.0E-06			
NNW-2	2.0E-06	20	3.3E-06	4.3E-07	1.0E-04	1.0E-04	10.0	1.0E-03	2.0E-05	1.00E-05	20	2.0E-04	1.4E-05	1.0E-06			
NNW-3	1.9E-06	20	-	1.9E-06	1.2E-05	-	-	-	2.0E-05	6.70E-06	20	1.3E-04	5.7E-06	1.9E-06			
NNW-4	9.2E-06	10	2.4E-05	1.2E-06	9.2E-06			1.2E-03	1.0E-05	6.52E-05	10	6.5E-04	1.5E-05	1.3E-06			
NNW-4_part						1.0E-04	20.0	2.0E-03									
NNW-4_part						1.0E-04	0.1	1.0E-05									
NNW-4_part						1.0E-04	1.0	1.0E-04									
NNW-4_part						1.0E-04	10.0	1.0E-03									
NNW-4_part						1.0E-04	30.0	3.0E-03									
NNW-5	3.1E-07	20	4.3E-07	5.3E-07	1.0E-06	-	-	-	2.0E-05	5.00E-06	20	1.0E-04	1.8E-06	1.0E-06			
NNW-6	1.4E-06	20	1.1E-06	1.4E-06	1.4E-06	-	-	-	2.0E-05	5.05E-06	20	1.0E-04	4.7E-06	1.4E-06			
NNW-7	6.2E-07	20	6.7E-06	6.4E-07	1.0E-06	1.0E-04	10.0	1.0E-03	2.0E-05	5.00E-06	20	1.0E-04	2.8E-06	1.0E-06			
NNW-8	1.1E-06	20	1.0E-06	-	1.1E-06	-	-	-	2.0E-05	5.00E-06	20	1.0E-04	6.8E-06	1.0E-06			
'Mystery feature"													5.4E-06				
SFZ01	4.3E-07	20				-	-	-						1.0E-06			
SFZ02	6.7E-06	20				-	-	-						6.7E-06			
SFZ03	4.3E-07	20	4.3E-07	-	-	-	-	-					2.2E-06	1.0E-06			
SFZ04	4.3E-07	20	4.3E-07	-	-	-	-	-						1.0E-06			
SFZ05	6.7E-06	20	1.2E-05	-	-	-	-	-						2.4E-05			
SFZ06	4.3E-07	20				-	-	-						1.0E-06			
SFZ07	4.3E-07	20	1.9E-06			-	-	-									
SFZ07_perpend																	
SFZ08	4.3E-07	20				-	-	-						1.0E-06			
SFZ09	4.3E-07	20				-	-	-						1.0E-06			
SFZ10	6.7E-06	20				-	-	-						6.7E-06			
SFZ11	4.9E-07	20	4.3E-07	4.9E-07	1.0E-06	-	-	-		5.00E-06	20	1.0E-04	2.4E-06	1.0E-06			
SFZ12	6.7E-06	20	1.6E-05			-	-	-						1.2E-05			
SFZ13	4.3E-07	20				-	-	-						1.0E-06			
SFZ14	4.3E-07	20	4.3E-07		1.0E-06								2.2E-06	1.0E-06			
SFZ14a_part				-	1.0E-06	-	-	-									
SFZ14b_part				-	1.0E-06	-	-	-									
SFZ15	6.7E-06	20				-	-	-						6.7E-06			

(a) : "xxxx_parall" indicates that the fracture zone has been divided into several parallell planes by the modeller. The total (added) tranmissivity for fracture zone is in row "xxxx"

"xxxx_part": indicates that the fracture zone has been divided into several parts by the modeller.The tranmissivity for fracture zone is in row "xxxx"

"xxxx_perpend": Transmissivity perpendicular to fracture zone plane

"xxxx": Transmissivity as single value or mean of "xxxx_part" or sum of "xxxx_parall"

(b) : TR 97-06, Table A2-7, Section 6.2.3, Section 6.3.3.

(c) : TR 97-06, Table A2-6

(d) : S not included in the model. The transient behavior is only based on the porosity of the system and not the compressibilty

Hydraulic Conductor Domain (HDR) (a)	Proposed (b) ne	Proposed (c)(d) width	ANDRA / ANTEA ne (d)	ANDRA / CEA ne (e)	ANDRA / ITASCA ne (d)		BMWi / BGR [width, m]	BMWi / BGR ne	CRIEPI ne (d)		ENRESA / UDC width	ENRESA / UDC ne	JNC / GOLDER ne	POSIVA / VTT ne	SKB /CFE / Intera (1) ne	SKB /CFE / Intera (2) ne	Compared features
	(-)	(m)	(-)	(-)	(-)			(-)	(-)			(-)	(-)	(-)	(-)	(-)	
EW-1N	1E-04	30		-	1E-04		10.0	2.5E-05	5E-05		30	1.1E-04	5E-04		3.7E-05	3.7E-05	▨
EW-1S	8E-04	30		1E-04	8E-04		10.0	2.5E-05	5E-04		30	8.4E-04	2E-03		1.9E-04	1.9E-04	▨
EW-1S+N			5E-04														
EW-1_perpend																	
EW-3	2E-03	15	2E-03	3E-04	2E-03			2.5E-05	1E-03		15	1.0E-02	4E-03		3.8E-04	3.8E-04	▨
EW-3_part							5.0	2.5E-05									
EW-3_part							10.0	2.5E-05									
EW-3_part							0.1	2.5E-05									
EW-3_part							1.0	2.5E-05									
EW-7	4E-03	10	-	4E-04	4E-03		-	-	1E-03		10	2.0E-03	1E-02		4.3E-04	4.3E-04	▨
NE-1	7E-03	30	6E-03	6E-04	7E-03		35.0	2.5E-05	5E-03		30	7.0E-03	7E-03		1.3E-03	1.3E-03	▨
NE-2	2E-04	5	1E-02	2E-04	5E-03			2.5E-05	6E-05		5	1.6E-04	2E-03		1.0E-04	1.0E-04	▨
NE-2_part							10.0	2.5E-05									
NE-2_part							0.1	2.5E-05									
NE-2_part							1.0	2.5E-05									
NE-2_part							10.0	2.5E-05									
NE-2_part							30.0	2.5E-05									
NE-3	4E-03	50	7E-03	4E-04	4E-03		35.0	2.5E-05	4E-03		50	2.5E-03	4E-03		2.1E-03	2.1E-03	▨
NE-4	9E-04	40	4E-03	2E-04	1E-03		35.0	2.5E-05	9E-04			8.5E-04	2E-03		6.3E-04	6.3E-04	▨
NE-4N_parall					9E-04						40	8.5E-04					
NE-4N_parall					9E-04						40	8.5E-04					
NW-1	5E-05	10	8E-05	-	5E-05		-	-	1E-04		10	5.0E-04	5E-04		6.0E-05	6.0E-05	▨
NNW-1	7E-04	20	7E-04	5E-05	1E-04		-	-	6E-04		20	8.0E-04	2E-03		2.1E-04	2.1E-04	▨
NNW-2	3E-03	20	2E-03	9E-05	2E-03		10.0	2.5E-05	1E-03		20	5.0E-03	5E-03		3.8E-04	3.8E-04	▨
NNW-3	1E-03	20	-	2E-04	6E-03		-	-	1E-03		20	1.0E-03	3E-03		5.0E-04	5.0E-04	▨
NNW-4	8E-03	10	2E-02	4E-04	8E-03			2.5E-05	4E-03		10	1.0E-03	2E-02		9.2E-04	9.2E-04	▨
NNW-4_part							20.0	2.5E-05									
NNW-4_part							0.1	2.5E-05									
NNW-4_part							1.0	2.5E-05									
NNW-4_part							10.0	2.5E-05									
NNW-4_part							30.0	2.5E-05									
NNW-5	2E-04	20	3E-04	1E-04	2E-04		-	-	3E-04		20	2.0E-03	9E-04		2.1E-04	2.1E-04	▨
NNW-6	8E-04	20	6E-04	2E-04	8E-04		-	-	8E-04		20	8.0E-04	2E-03		4.1E-04	4.1E-04	▨
NNW-7	4E-04	20	4E-03	1E-04	4E-04		10.0	2.5E-05	9E-04		20	1.0E-03	1E-03		5.0E-04	5.0E-04	▨
NNW-8	6E-04	20	6E-04	-	6E-04	-	-	-	6E-04		20	1.0E-03	2E-03		3.2E-04	3.2E-04	▨
'Mystery feature"		20											2E-03				
SFZ01	3E-04	20				-	-	-									▨
SFZ02	4E-03	20				-	-	-									▨
SFZ03	3E-04	20	3E-04	-	-	-	-	-					1E-03		1.80E-04	1.80E-04	▨
SFZ04	3E-04	20	3E-04	-	-	-	-	-									▨
SFZ05	4E-03	20	6E-03	-	-	-	-	-									▨
SFZ06	3E-04	20				-	-	-									▨
SFZ07	3E-04	20	1E-03			-	-	-							1.80E-04	1.80E-04	▨
SFZ07_perpend																	
SFZ08	3E-04	20				-	-	-									▨
SFZ09	3E-04	20				-	-	-									▨
SFZ10	4E-03	20				-	-	-									▨
SFZ11	3E-04	20	3E-04	1E-04	3E-04	-	-	-			20	3.4E-04	1E-03		1.80E-04	1.80E-04	▨
SFZ12	4E-03	20	8E-03			-	-	-							1.16E-03	1.16E-03	▨
SFZ13	3E-04	20				-	-	-									▨
SFZ14	3E-04	20	3E-04		3E-04								1E-03				▨
SFZ14a_part				-		-	-	-									
SFZ14b_part				-		-	-	-									
SFZ15	4E-03	20				-	-	-									▨

(a) : "xxxx_parall" indicates that the fracture zone has been divided into several parallell planes by the modeller. The total (added) tranmissivity for fracture zone is in row "xxxx"

"xxxx_part": indicates that the fracture zone has been divided into several parts by the modeller.The tranmissivity for fracture zone is in row "xxxx"

"xxxx_perpend": Transmissivity perpendicular to fracture zone plane

"xxxx": Transmissivity as single value or mean of "xxxx_part" or sum of "xxxx_parall"

(b) : TR 97-06, Table A2-7, Section 6.2.3, Section 8.3.2

(c) : TR 97-06, Table A2-6

(d) : TR 97-06, Section 8.3.2 ne based on equation for ne=f(K)

(e) : TR 97-06, Section 8.3.2 ne based on equation for transport apperture et=f(T)

Hydraulic Rock Domain (HRD)	Proposed Depth range (a)	Scale of measure ments (b)	Proposed K (Median) (b)	Proposed s(log10(K)) (b)	ANDRA / ANTEA	ANDRA / CEA (c)	ANDRA / ITASCA (c)	BMWi / BGR (c)	CRIEPI	ENRESA / UDC (c)	JNC / GOLDER	POSIVA / VTT	SKB /CFE / Intera (1) Scale of measure ments	SKB /CFE / Intera (1) K (Median)	SKB /CFE / Intera (1) s(log10(K))	SKB /CFE / Intera (2)
	(m)	(m)	(m/s)	(m/s)	(m/s)				(m/s)	(m/s)		(m/s)	(m)	(m/s)	(m/s)	
SRD 1	0-600	3	1.8E-09	1.32	1.00E-08	n	n	n	6.0E-09	n	DFN	1.58E-08	20	1.6E-08	0.7	K=f(DFN)
SRD 2	0-600	3	1.5E-08	1.8E+00	1.00E-08	n	n	n	6.0E-09	n	DFN	7.94E-08	20	1.6E-08	1.17	K=f(DFN)
SRD 3	0-600	3	3.4E-10	1.6E+00	1.00E-08	n	n	n	6.0E-09	n	DFN	2.00E-09	20	2.0E-09	1.01	K=f(DFN)
SRD 4	0-600	15	3.5E-07	1.6E+00	1.00E-07	n	n	n	6.0E-09	n	DFN	2.51E-08	20	2.5E-08	1.51	K=f(DFN)
SRD 1-4	600-db	300	4.7E-08	7.2E-01	1.00E-08	n	n	n	6.0E-09	n	DFN	9.30E-09	20	3.2E-09	1.61	K=f(DFN)
SRD 5	Fine-gr. Granite	3	4.8E-09	2.0E+00	1.00E-08	n	n	n	6.0E-09	n	DFN	9.30E-09	20	2.1E-08	1.37	K=f(DFN)

(a) : db = depth to bottom level of numerical model

(b) : TR 97-06, Table 6-21

(c) : n= HRD are not modelled

Hydraulic Rock Domain (HRD)	Proposed Depth range (a)	Proposed Ss (b)	ANDRA / ANTEA	ANDRA / CEA (c)	ANDRA / ITASCA (c)	BMWi / BGR (c)	CRIEPI	ENRESA / UDC (c)	JNC / GOLDER	POSIVA / VTT	SKB /CFE / Intera (1) (d)	SKB /CFE / Intera (2) (d)
	(m)	(m/s)	(m/s)	(m/s)	(m/s)	(m/s)	(m/s)	(m/s)		(m/s)		
SRD 1	0-600	Ss=f(K)	1.00E-06	n	n	n	1.0E-06	n	DFN	8.40E-07		
SRD 2	0-600	Ss=f(K)	1.00E-06	n	n	n	1.0E-06	n	DFN	8.40E-07		
SRD 3	0-600	Ss=f(K)	1.00E-06	n	n	n	1.0E-06	n	DFN	8.40E-07		
SRD 4	0-600	Ss=f(K)	3.00E-06	n	n	n	1.0E-06	n	DFN	8.40E-07		
SRD 1-4	600-db	Ss=f(K)	1.00E-06	n	n	n	1.0E-06	n	DFN	8.40E-07		
SRD 5	Fine-gr. Granite	Ss=f(K)	1.00E-06	n	n	n	1.0E-06	n	DFN	8.40E-07		

(a) : db = depth to bottom level of numerical model

(b) : TR 97-06, Table 6-17

(c) : n= HRD are not modelled

(d) : Ss not included in the model. The transient behavior is only based on the porosity of the system and not the compressibilty

Hydraulic Rock Domain (HRD)	**Proposed Depth range (a)**	**Proposed ne (b)**	**ANDRA / ANTEA**	**ANDRA / CEA (c)**	**ANDRA / ITASCA (c)**	**BMWi / BGR (c)**	**CRIEPI**	**ENRESA / UDC (c)**	**JNC / GOLDER**	**POSIVA / VTT (d)**	**SKB /CFE / Intera (1) (e)**	**SKB /CFE / Intera (2) (f)**
	(m)	**(-)**	**(-)**				**(-)**			**(-)**	**(-)**	**(-)**
SRD 1	0-600	ne=f(K)	3.3E-05	n	n	n	2.2E-05	n	DFN	4.60E-04	ne=f(K)	ne=f(DFN)
SRD 2	0-600	ne=f(K)	3.3E-05	n	n	n	2.2E-05	n	DFN	7.80E-04	ne=f(K)	ne=f(DFN)
SRD 3	0-600	ne=f(K)	3.3E-05	n	n	n	2.2E-05	n	DFN	2.30E-04	ne=f(K)	ne=f(DFN)
SRD 4	0-600	ne=f(K)	1.9E-04	n	n	n	2.2E-05	n	DFN	5.30E-04	ne=f(K)	ne=f(DFN)
SRD 1-4	600-db	ne=f(K)	3.3E-05	n	n	n	2.2E-05	n	DFN	3.80E-04	ne=f(K)	ne=f(DFN)
SRD 5	Fine-gr. Granite	ne=f(K)	3.3E-05	n	n	n	2.2E-05	n	DFN	3.80E-04	ne=f(K)	ne=f(DFN)

(a) : db = depth to bottom level of numerical model

(b) : TR 97-06, eq. 8-8.

(c) : n= HRD are not modelled

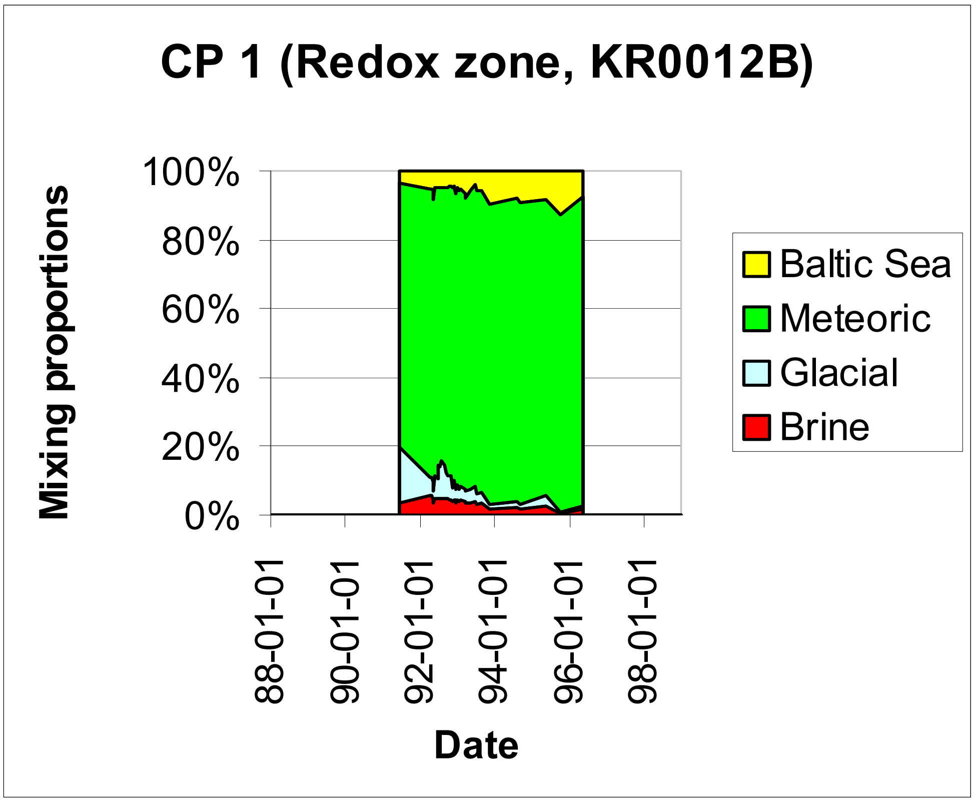
(d) : Flow porosity at surface. Decresing towards depth

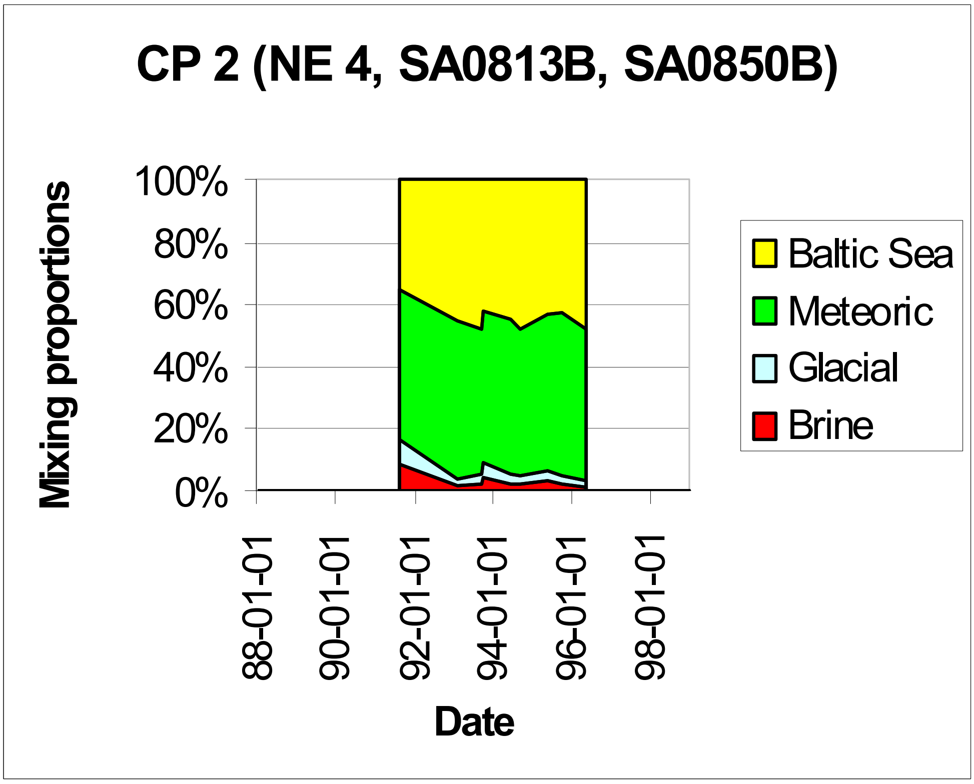
(e) : Flow porosity based on eq. 8-8 in TR 97-06 assum that ne<=0.05 giving a mean porosity of 4e-3 inthe total domain (HCD+HRD).

(f) : Flow porosity based on eq. 8-13 in TR 97-06 assum that ne<=0.05 giving a mean porosity of 4e-3.

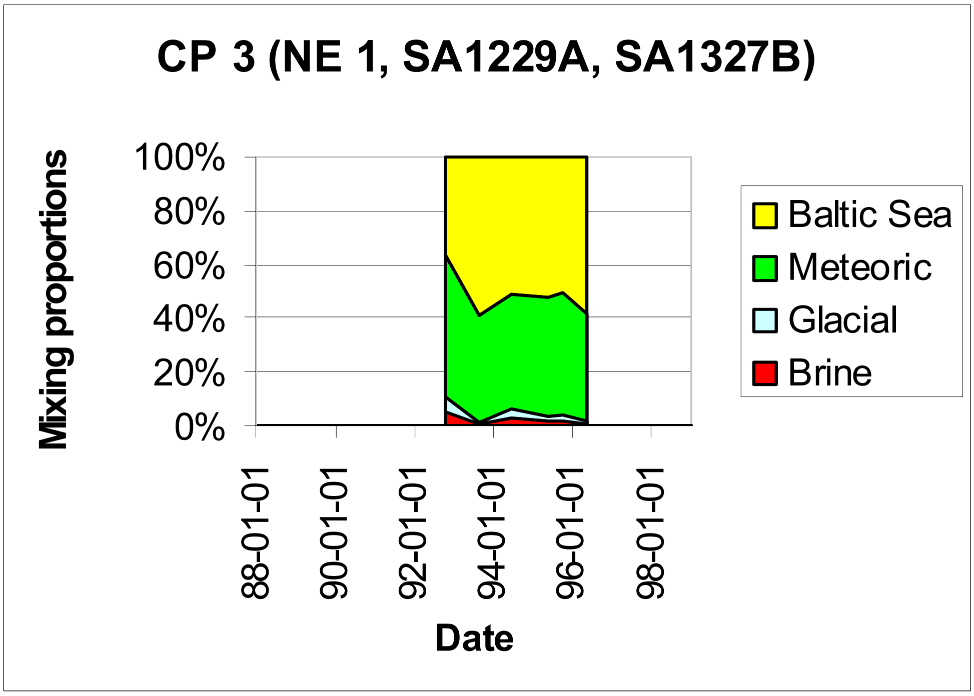
Appendix 6: Task 5. Measurements and predictions at control points

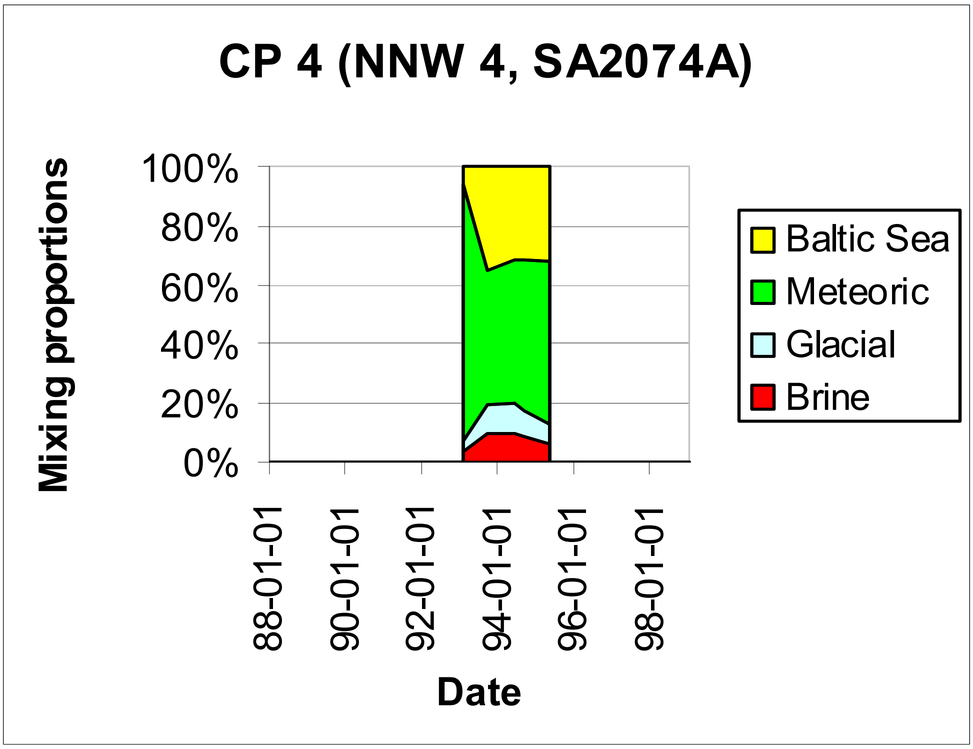
Mixing proportions based on measurements at control points and predictions of mixing proportions.



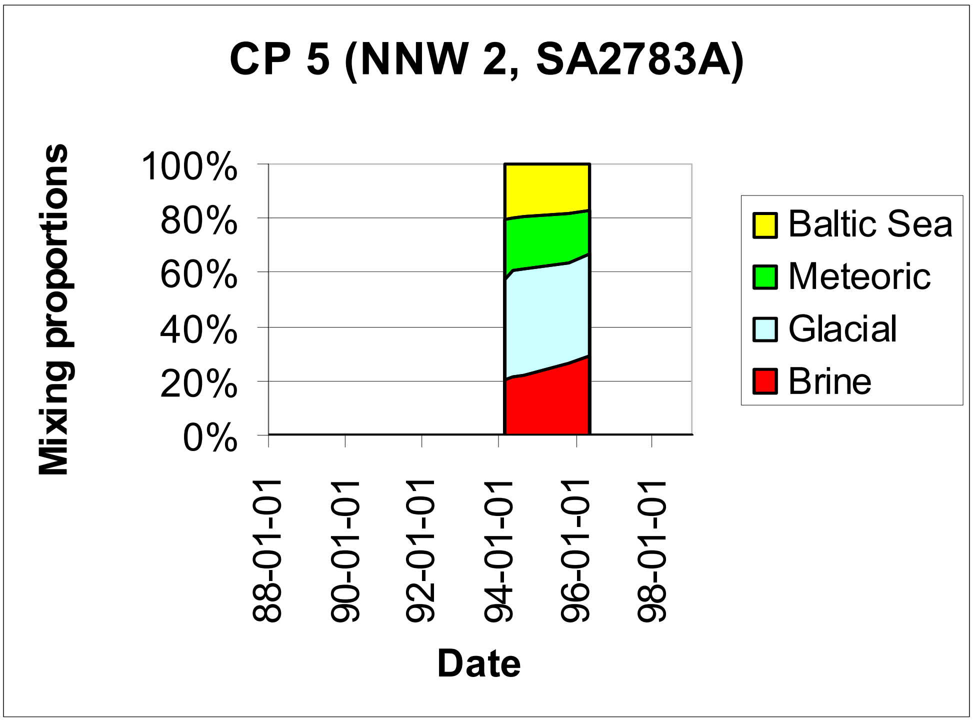


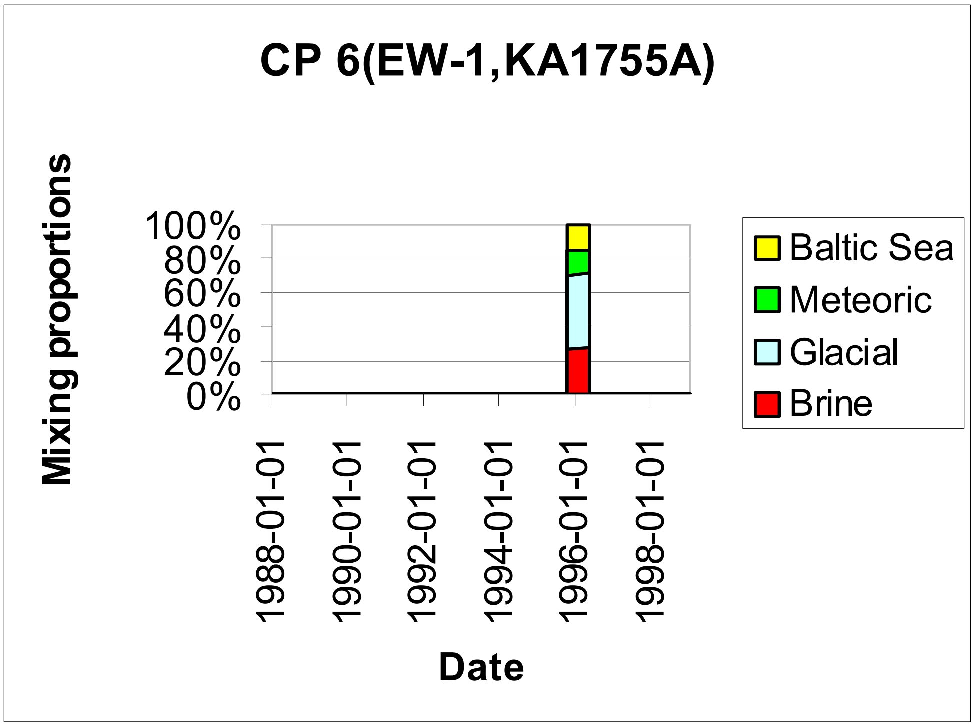
Task 5. Mixing proportions based on measurements at control points



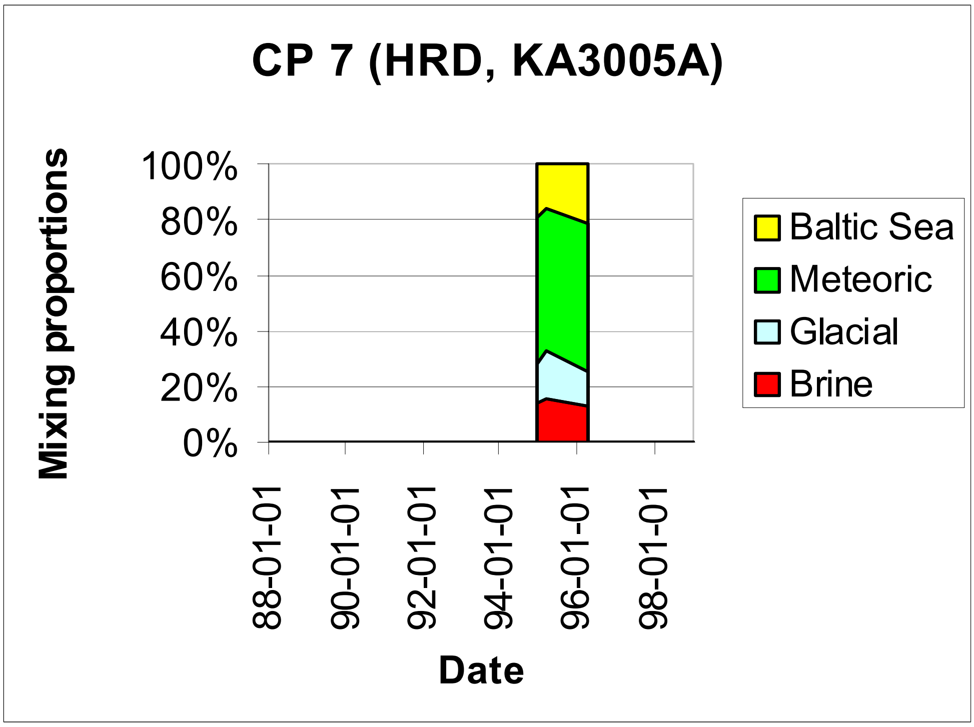


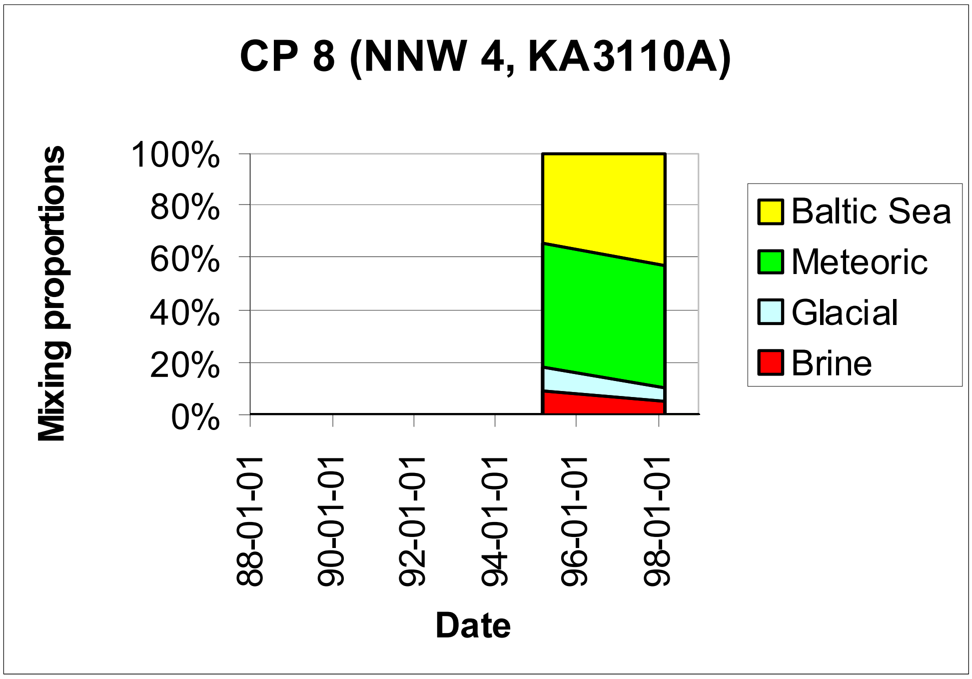
Task 5. Mixing proportions based on measurements at control points



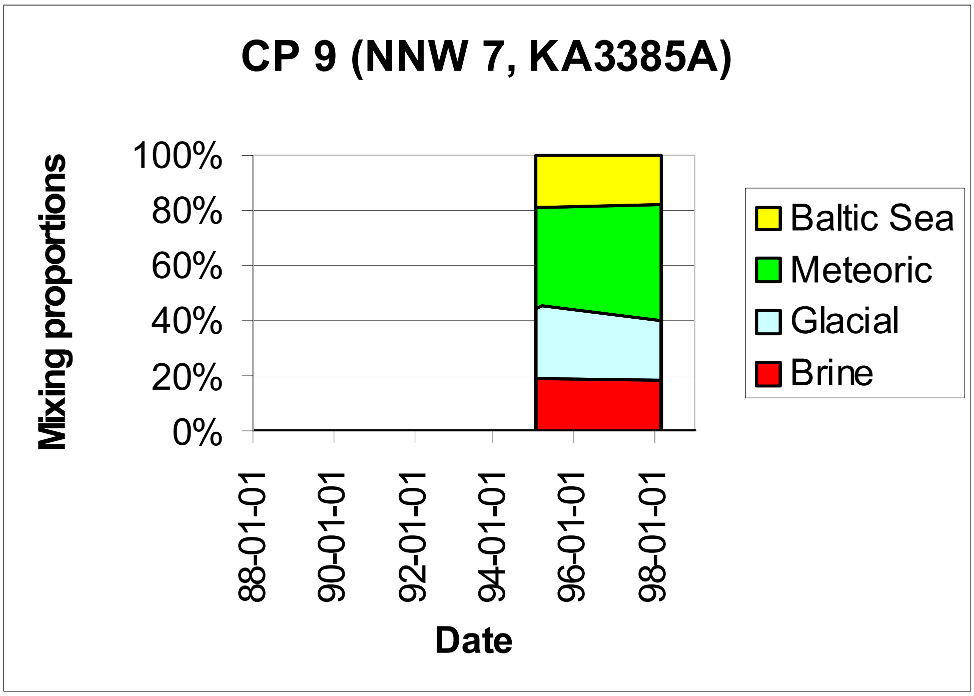


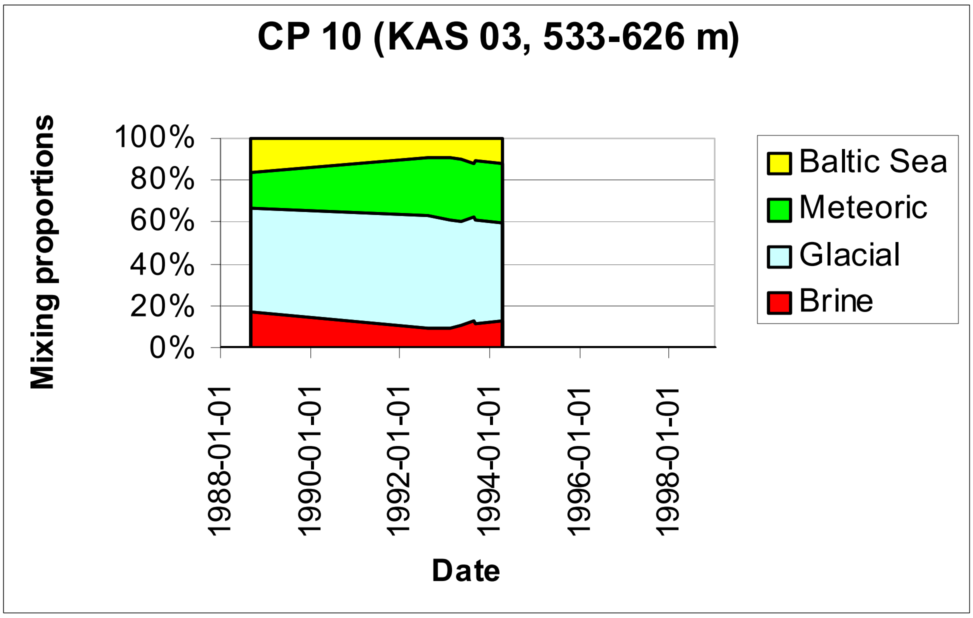
Task 5. Mixing proportions based on measurements at control points



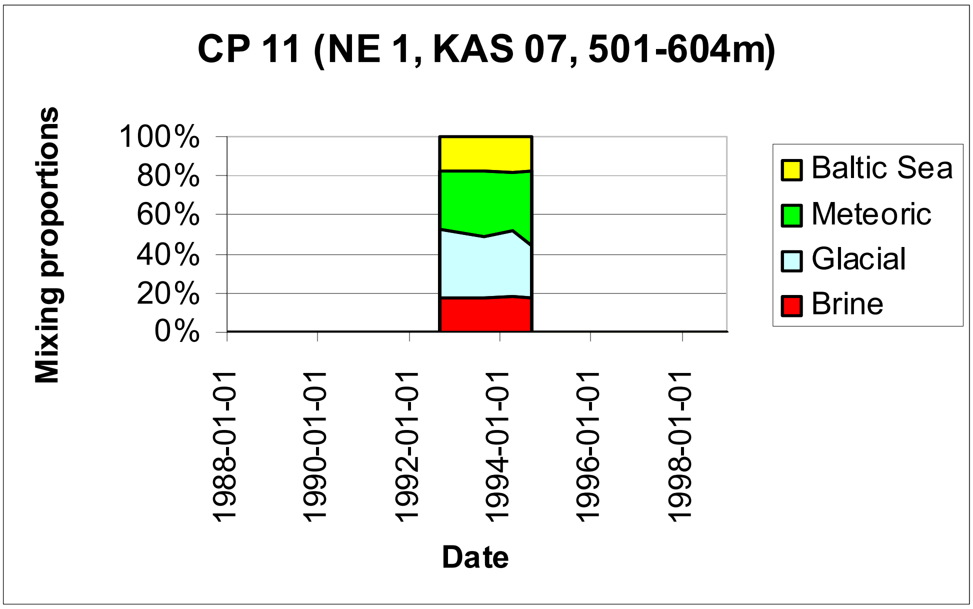


Task 5. Mixing proportions based on measurements at control points

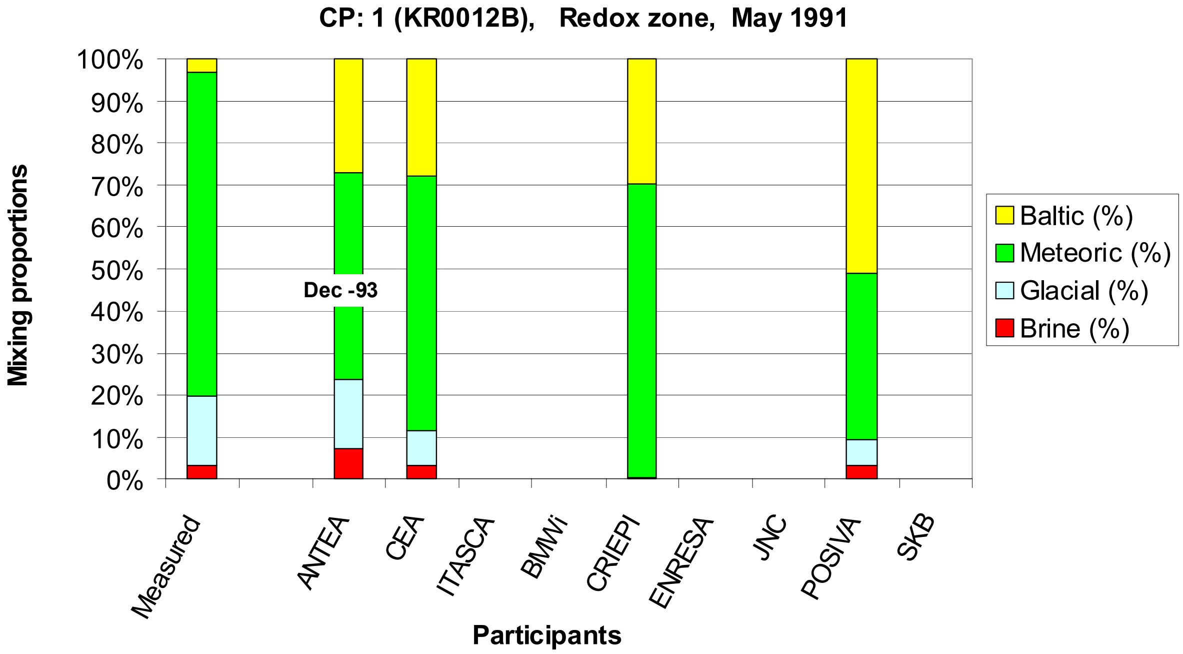


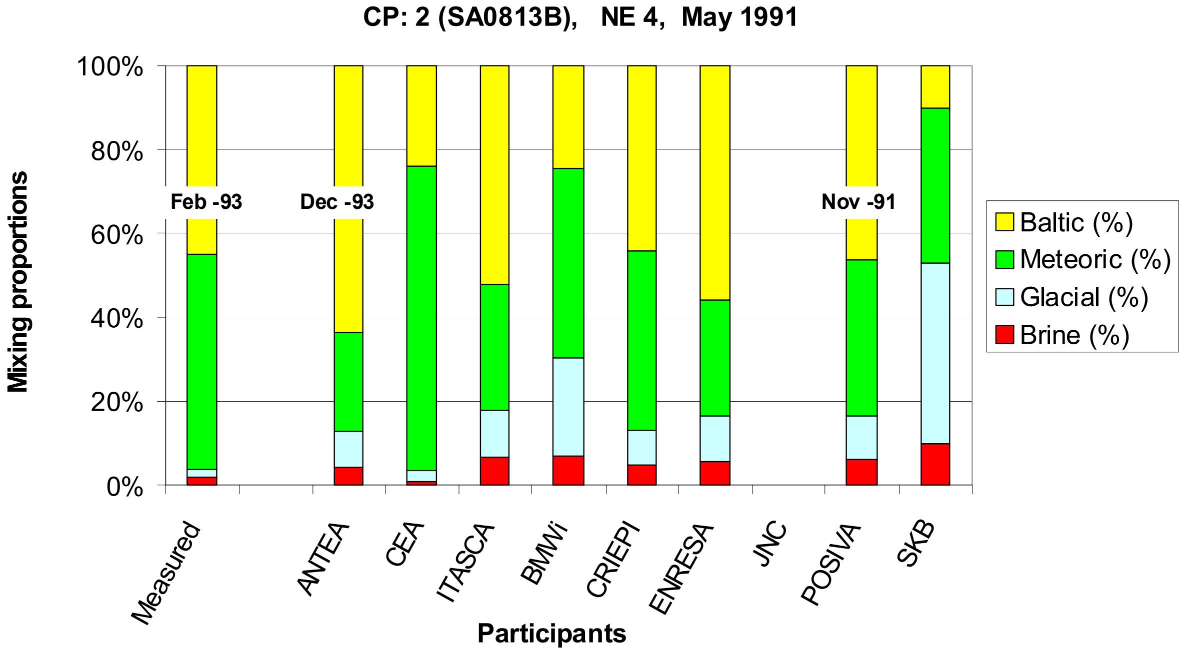


Task 5. Mixing proportions based on measurements at control points

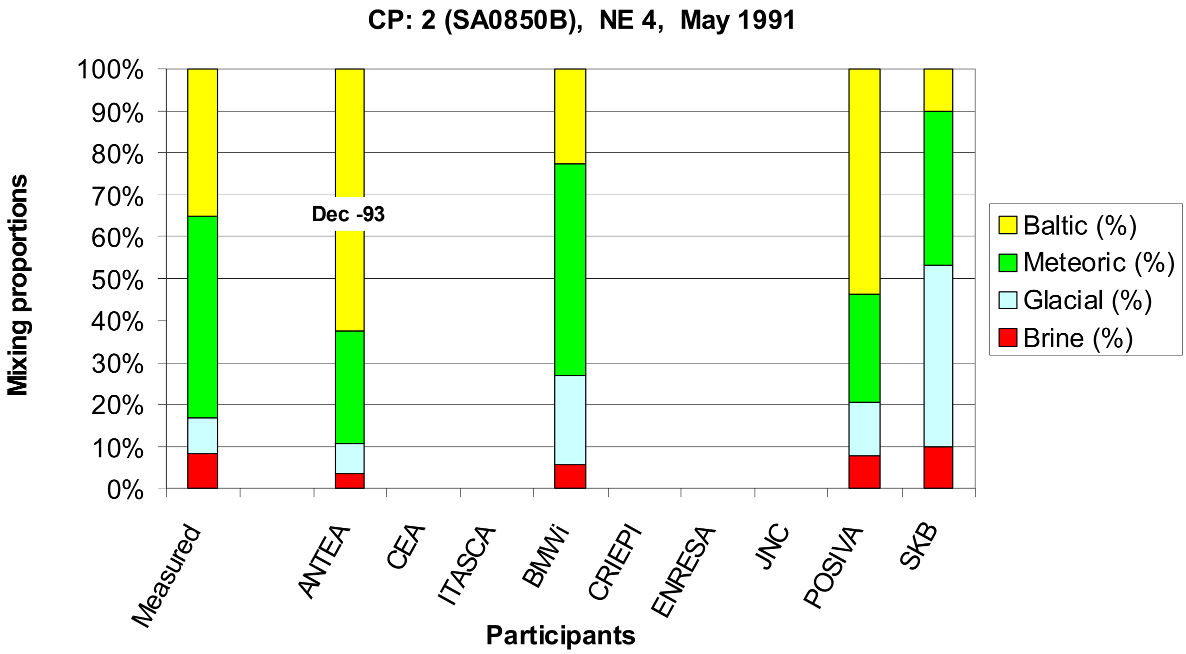


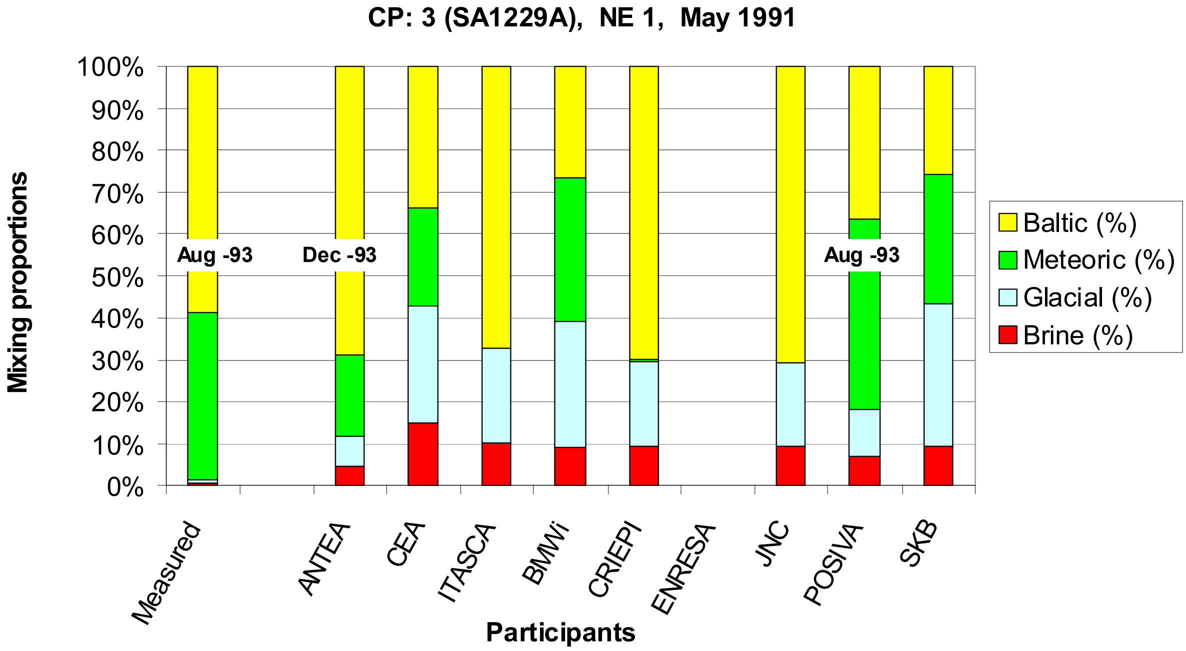
Task 5. Mixing proportions based on measurements at control points



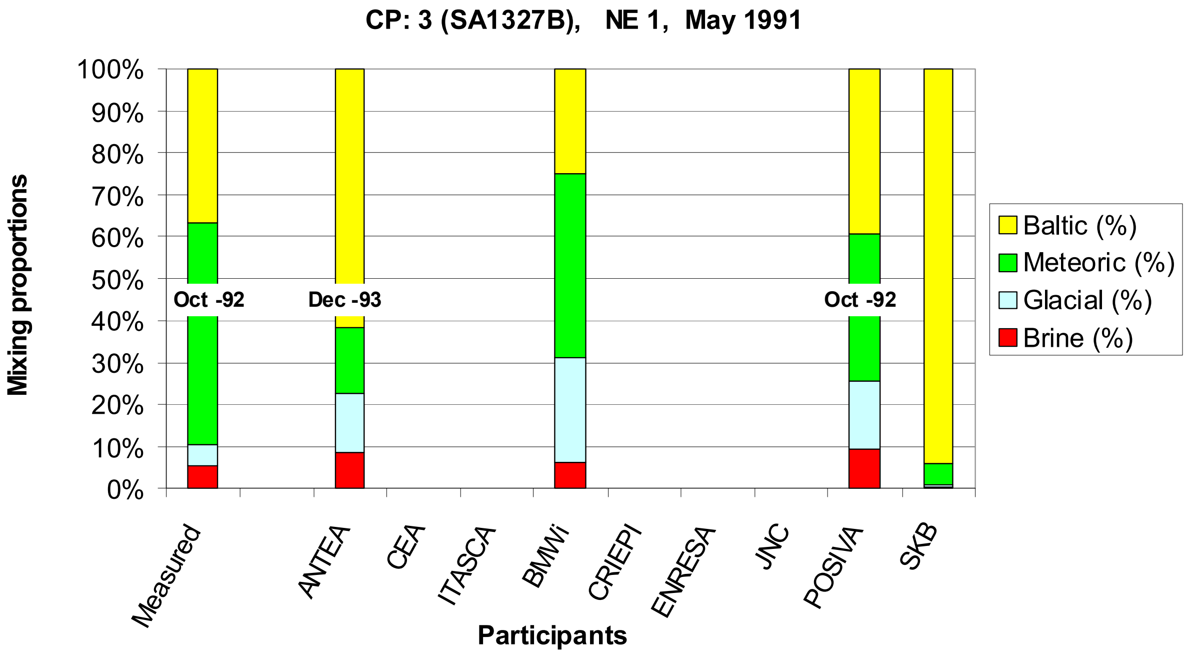


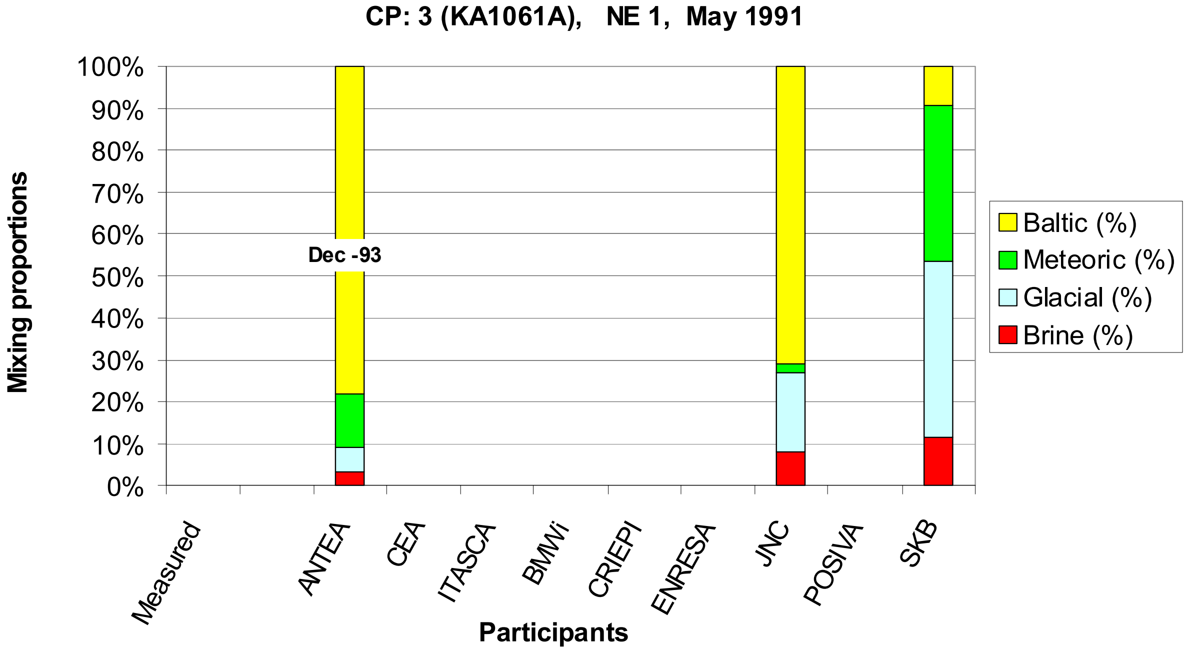
Task 5. Predictions of mixing proportions



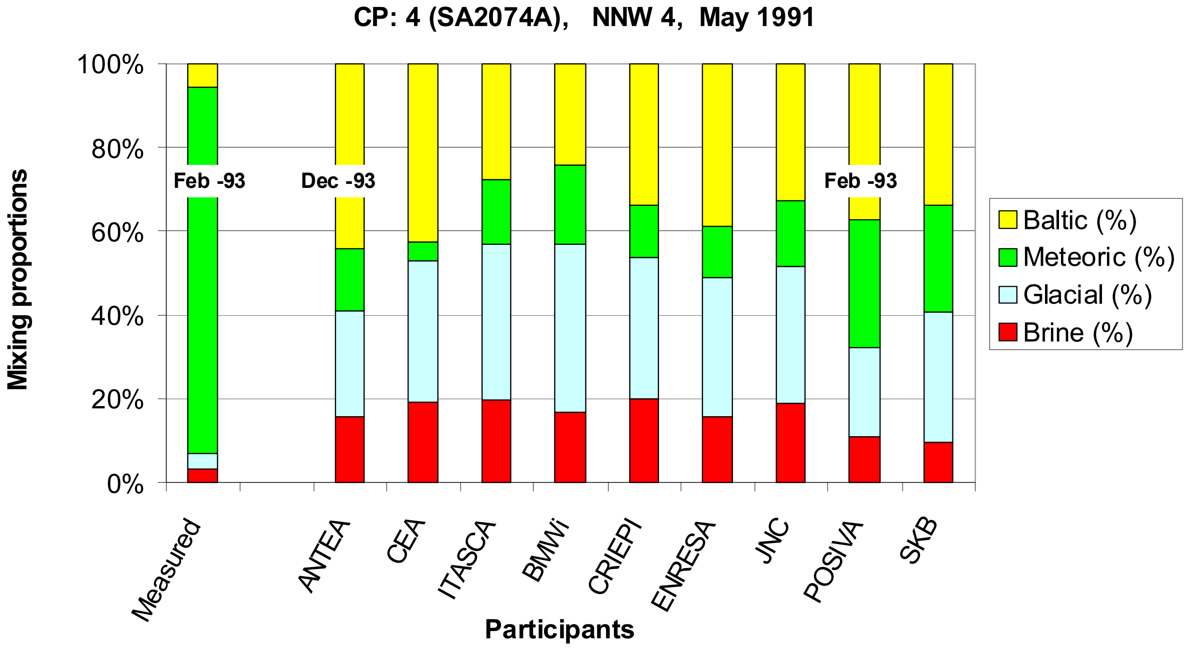


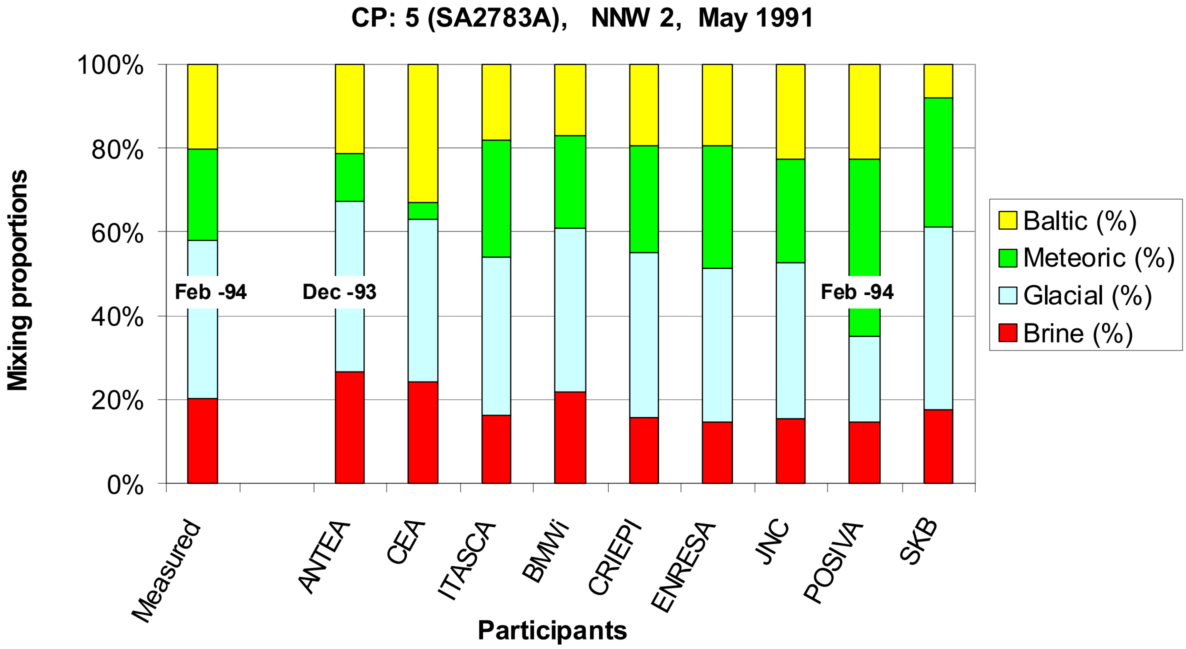
Task 5. Predictions of mixing proportions



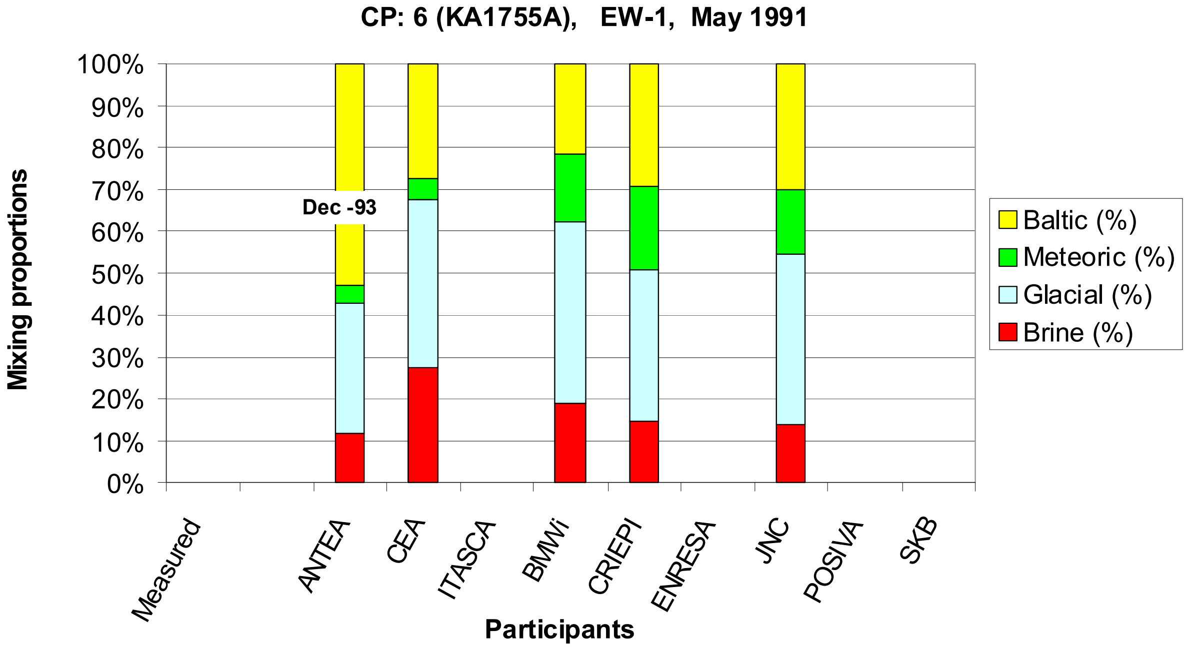


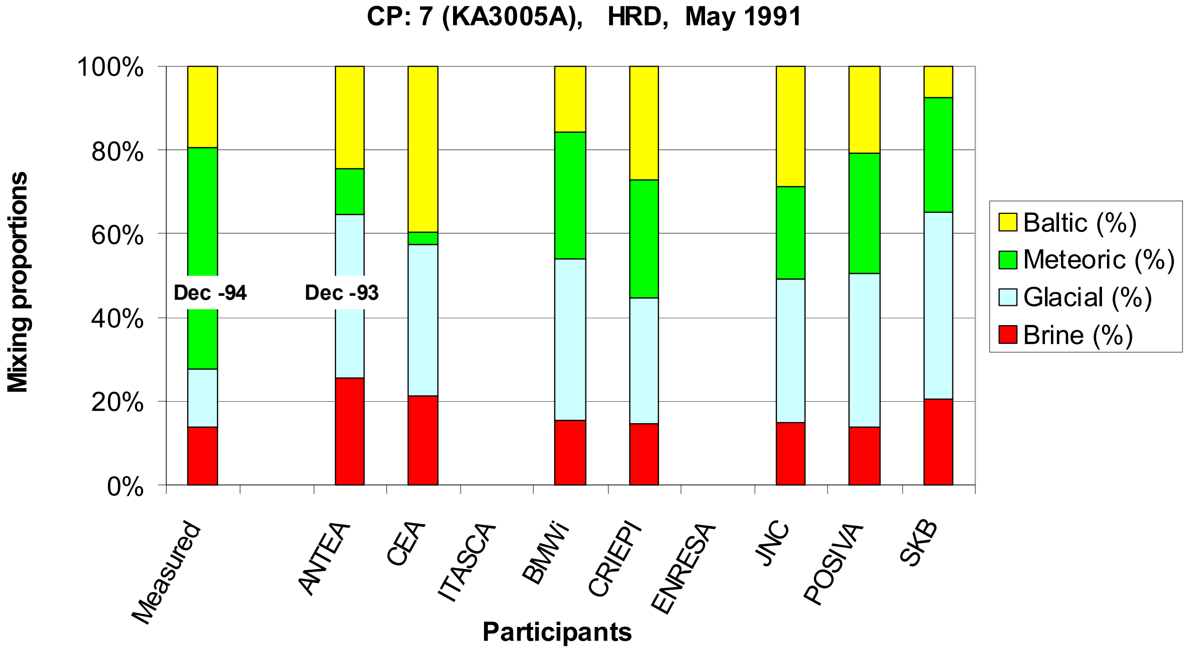
Task 5. Predictions of mixing proportions



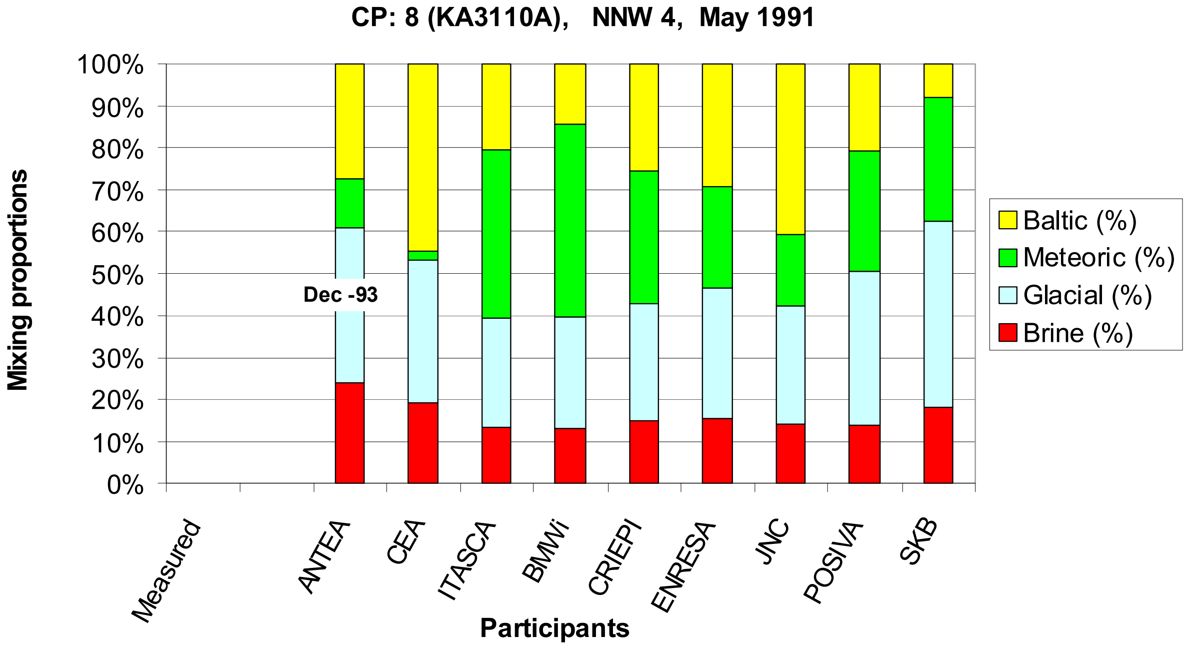


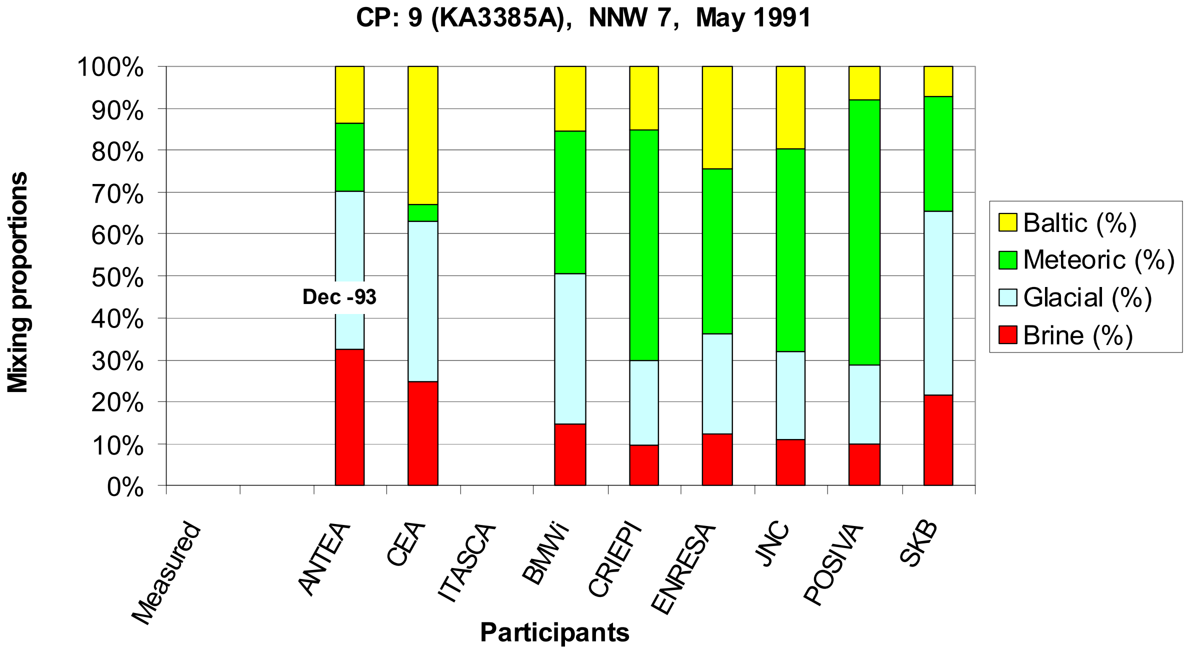
Task 5. Predictions of mixing proportions



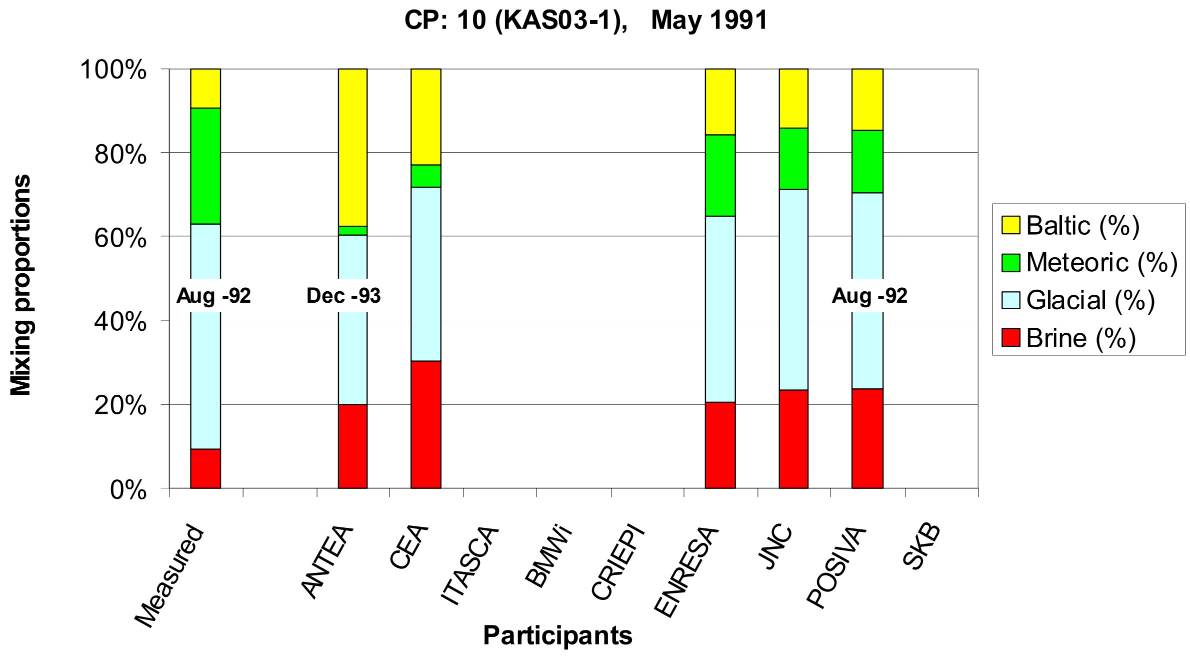


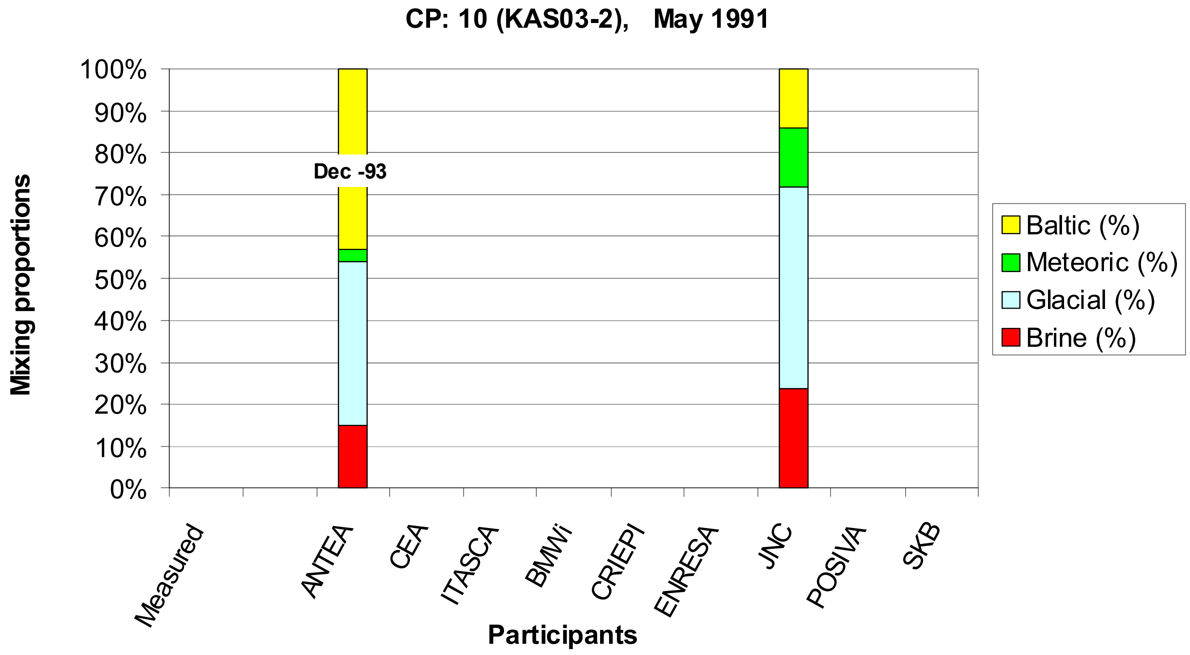
Task 5. Predictions of mixing proportions



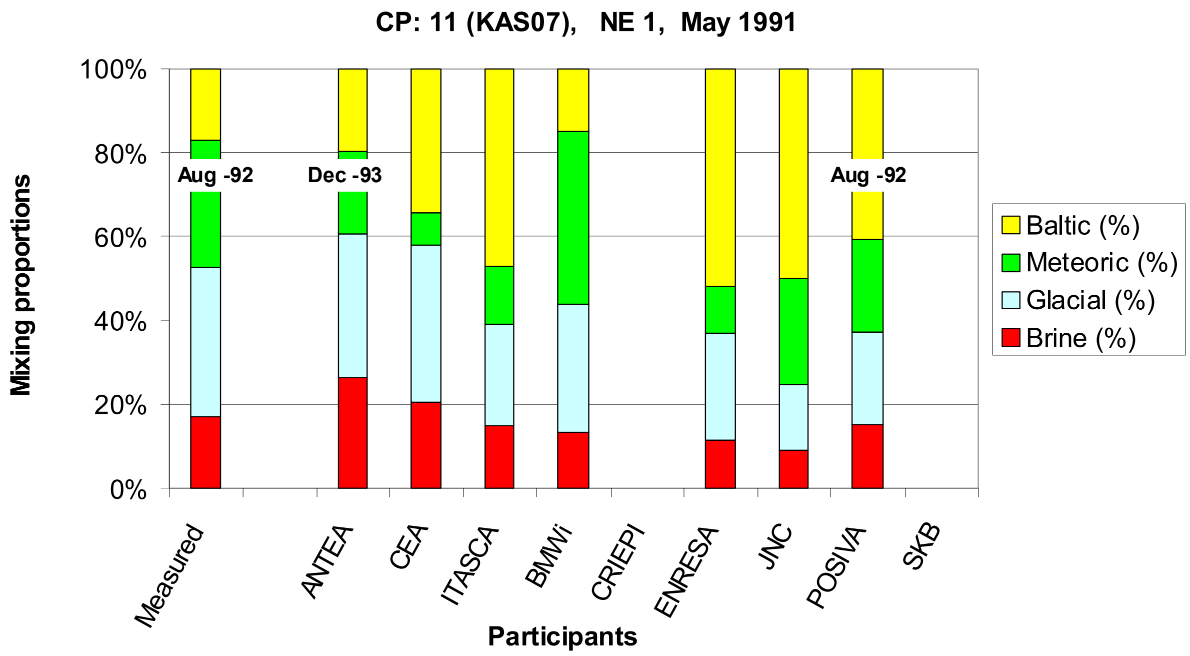


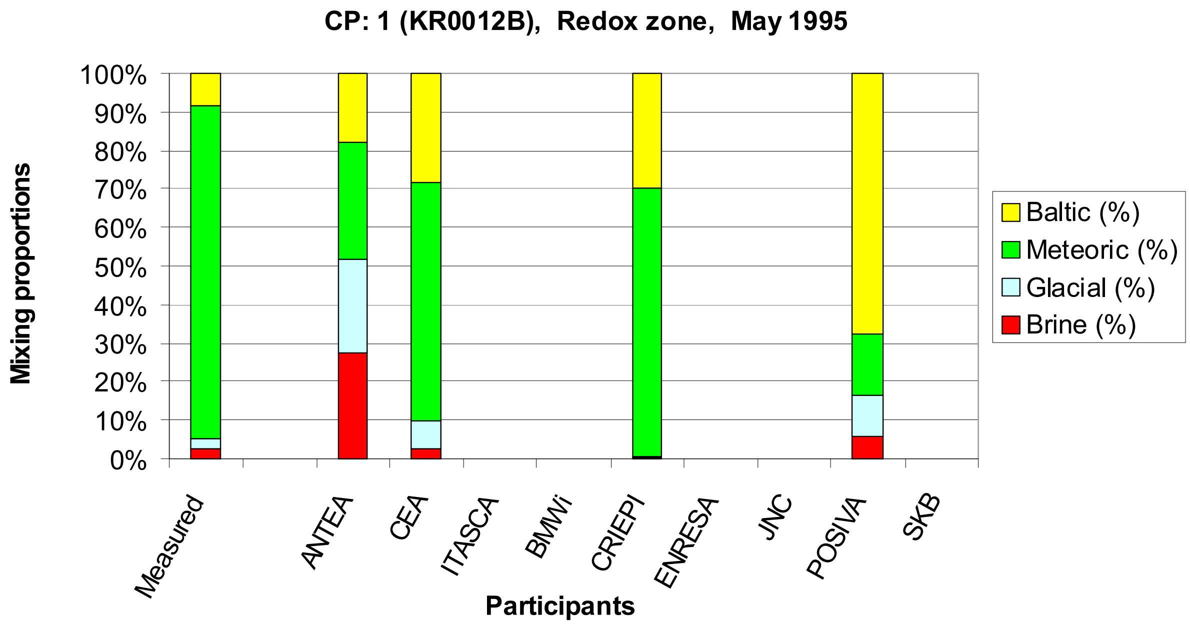
Task 5. Predictions of mixing proportions



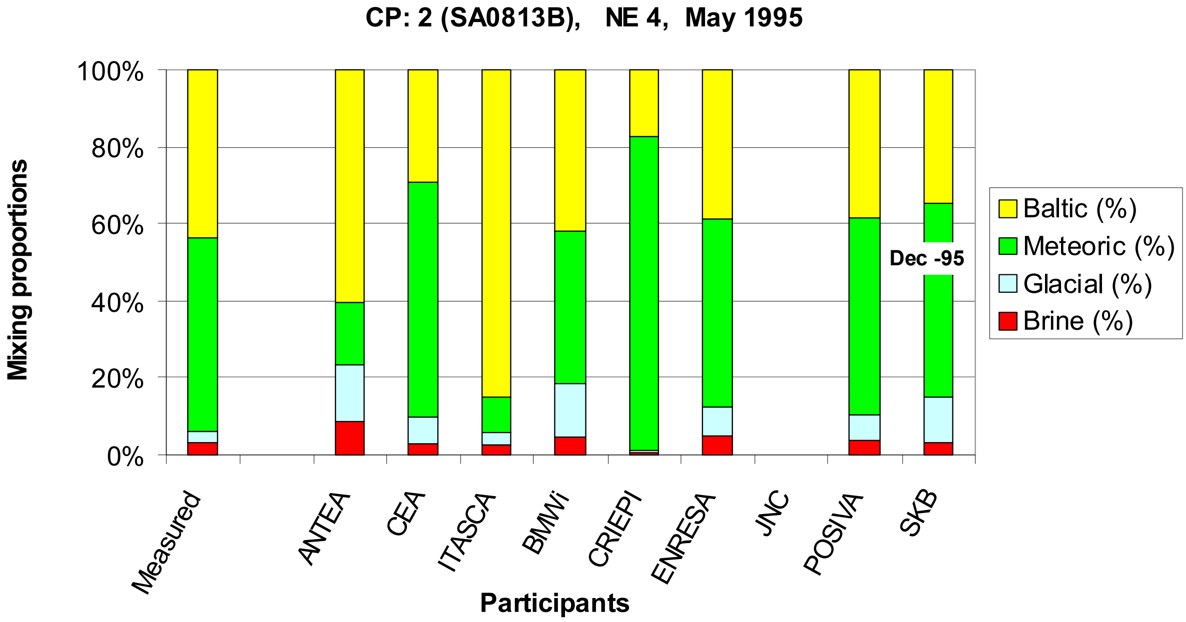


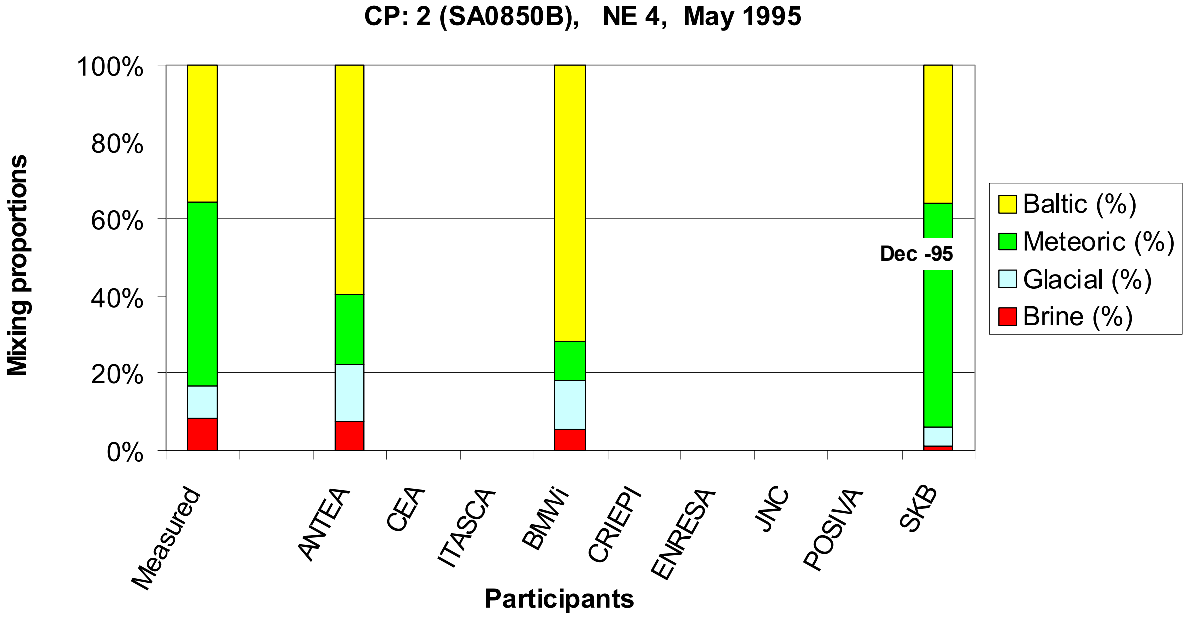
Task 5. Predictions of mixing proportions



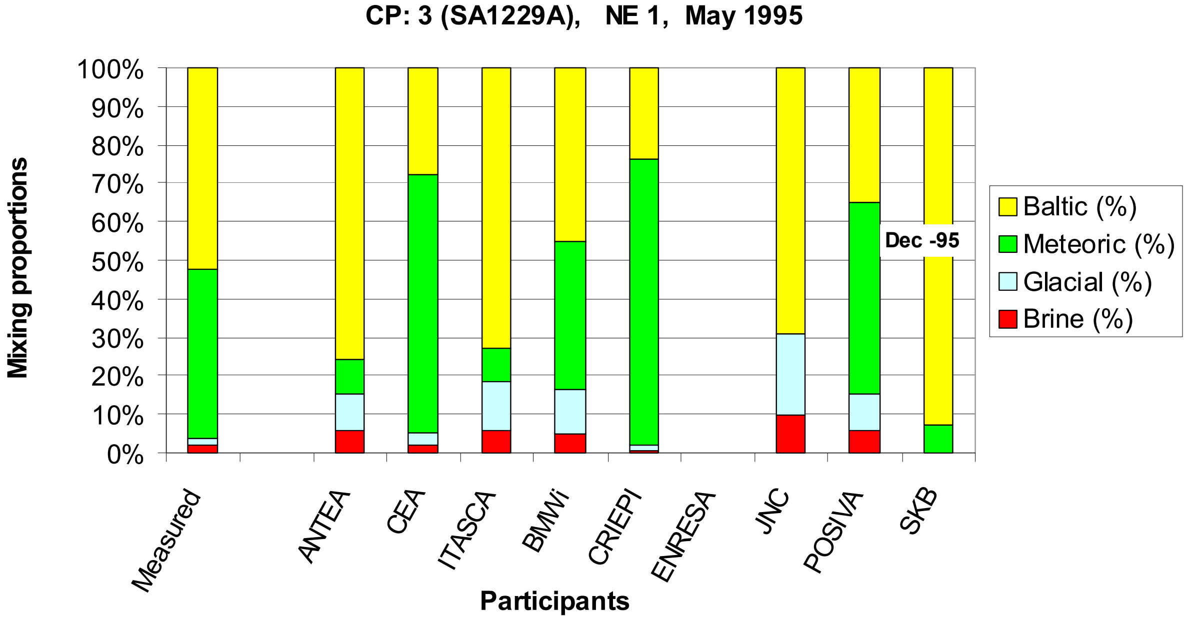


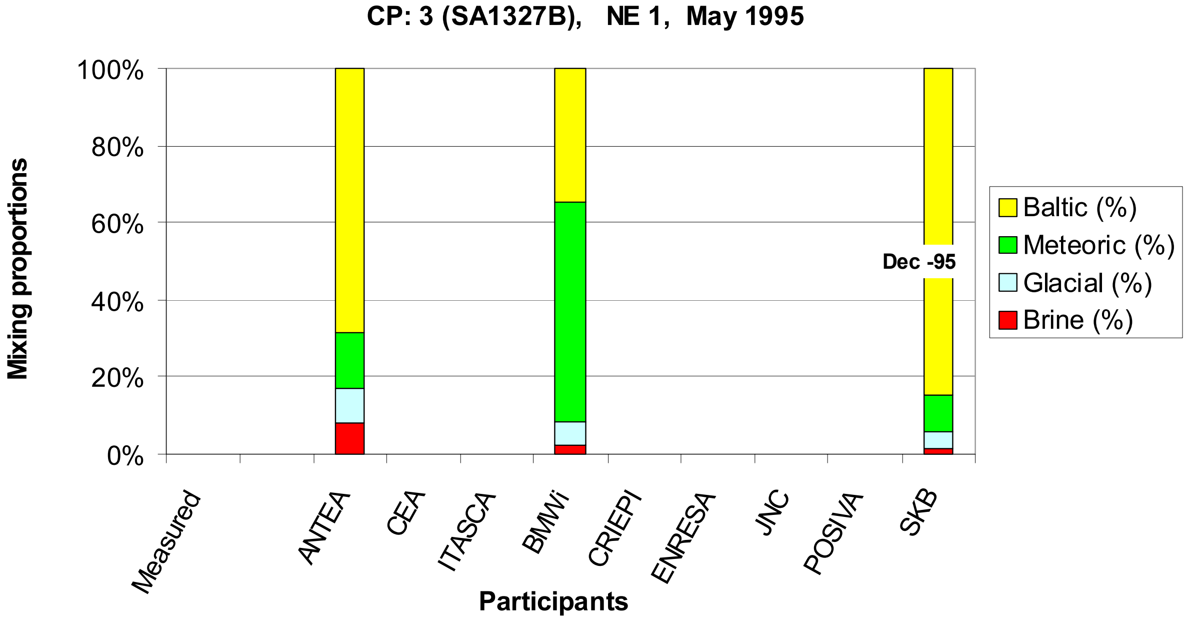
Task 5. Predictions of mixing proportions



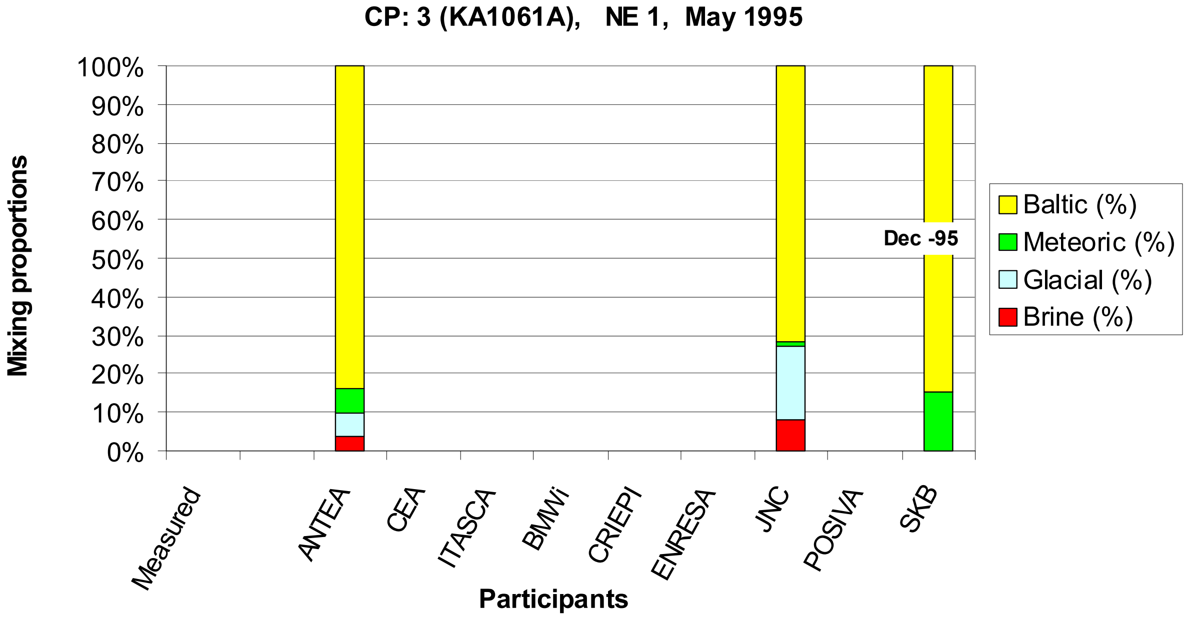


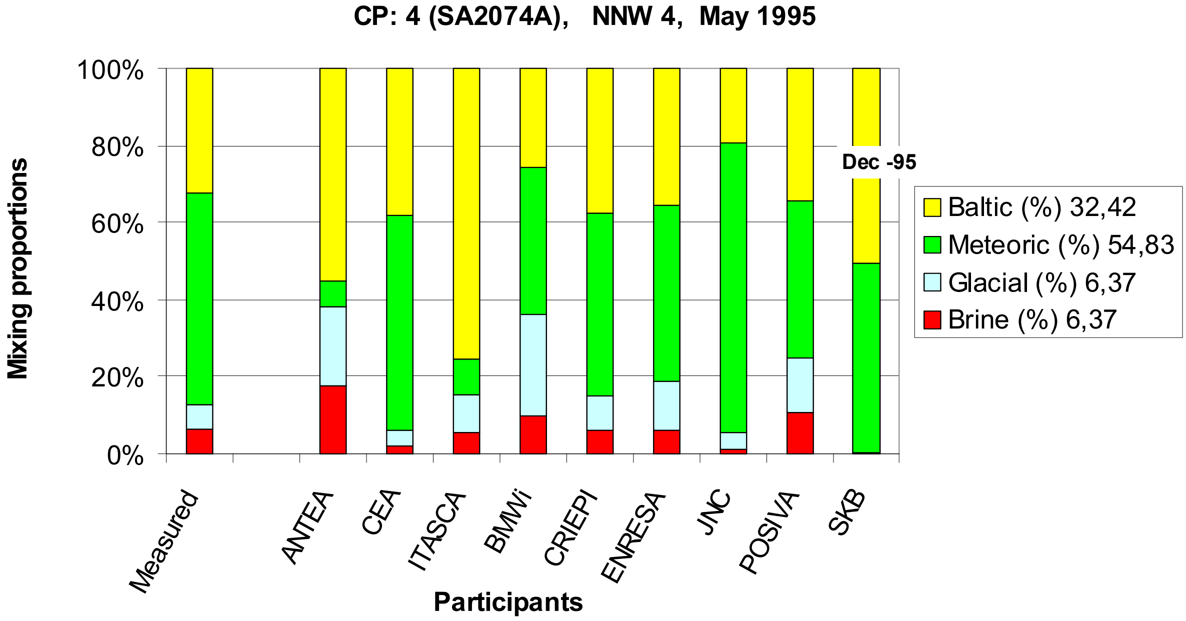
Task 5. Predictions of mixing proportions



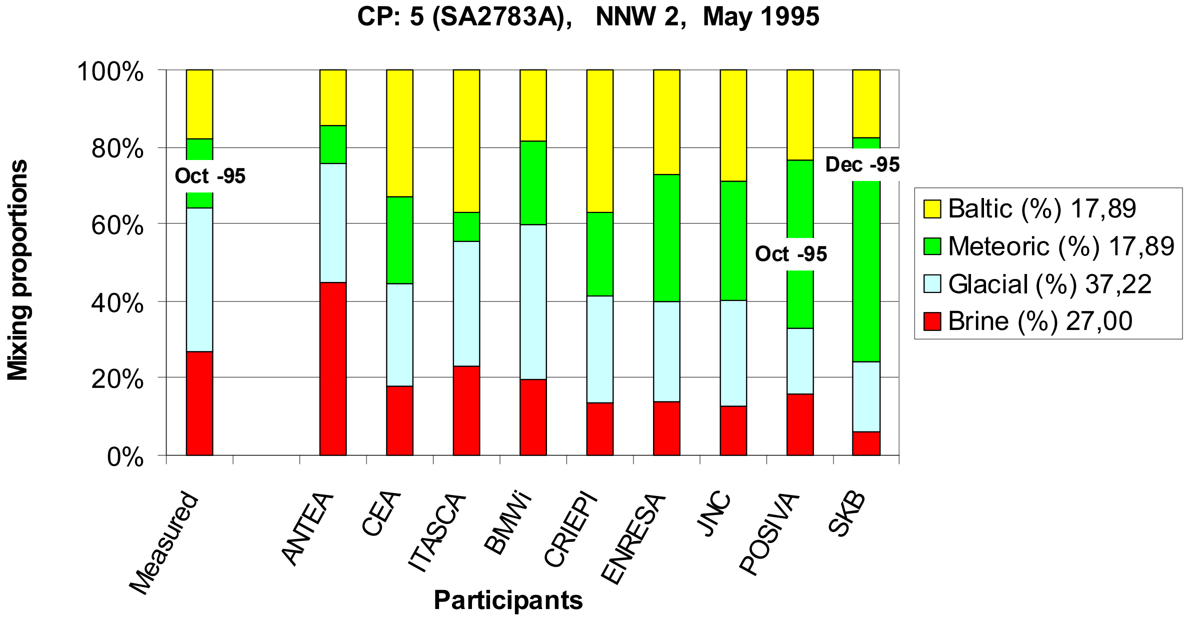


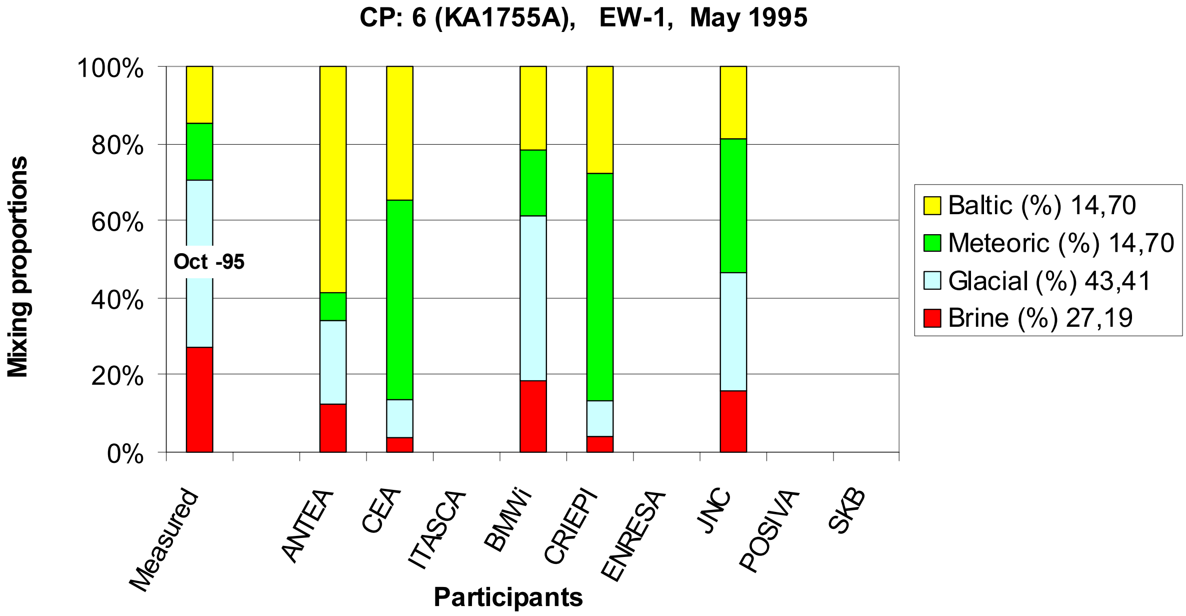
Task 5. Predictions of mixing proportions



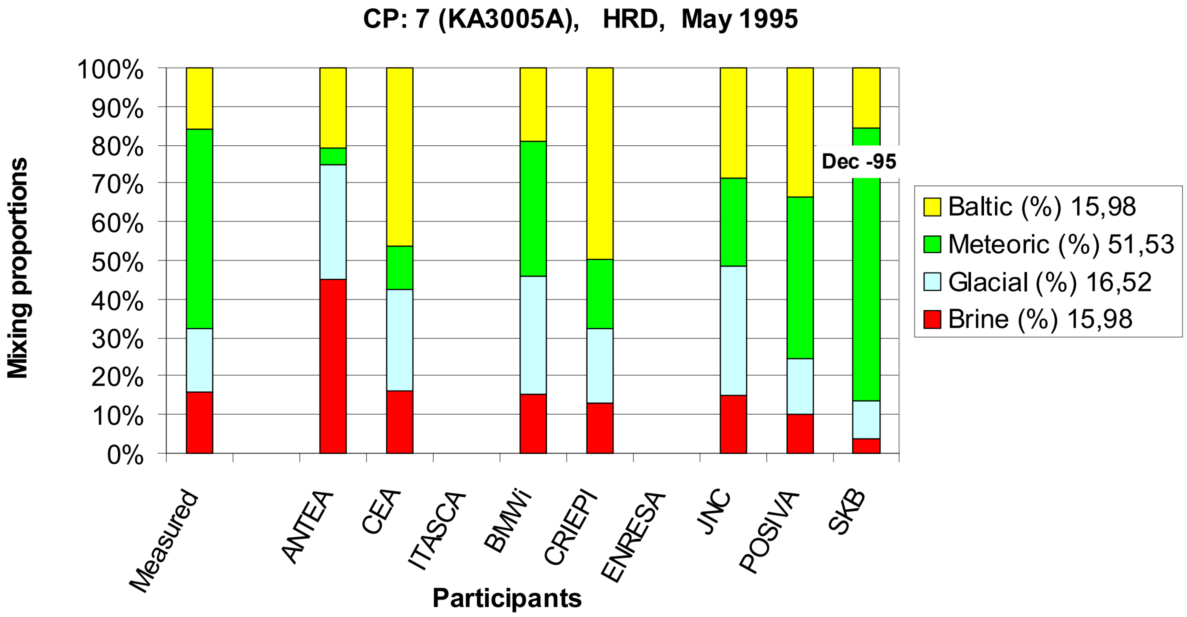


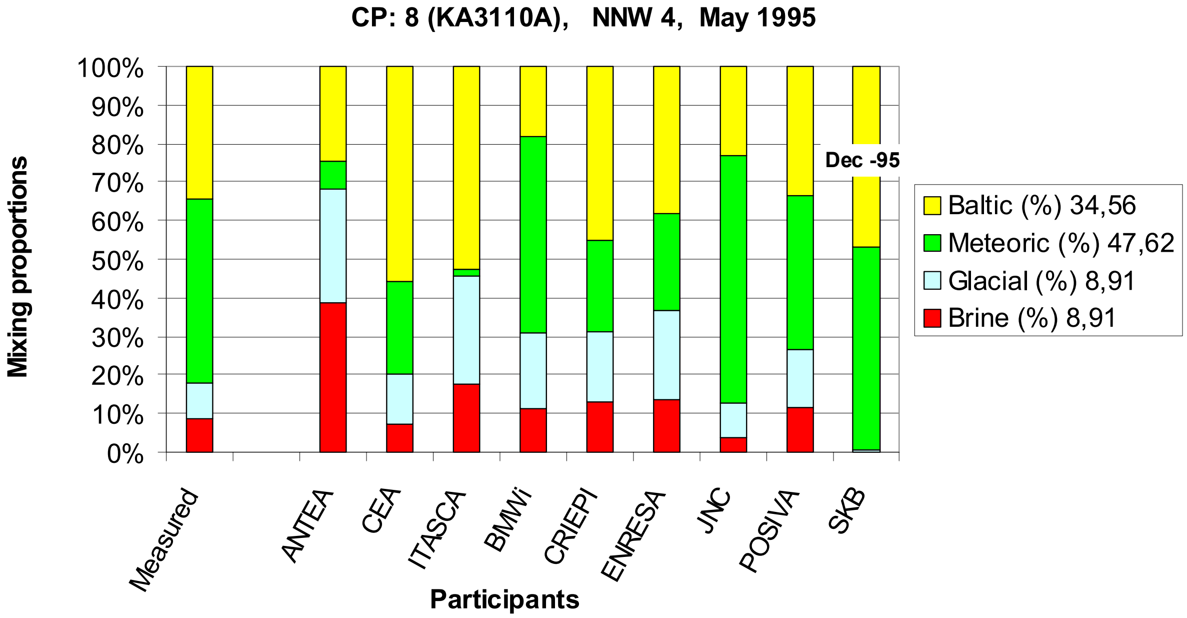
Task 5. Predictions of mixing proportions



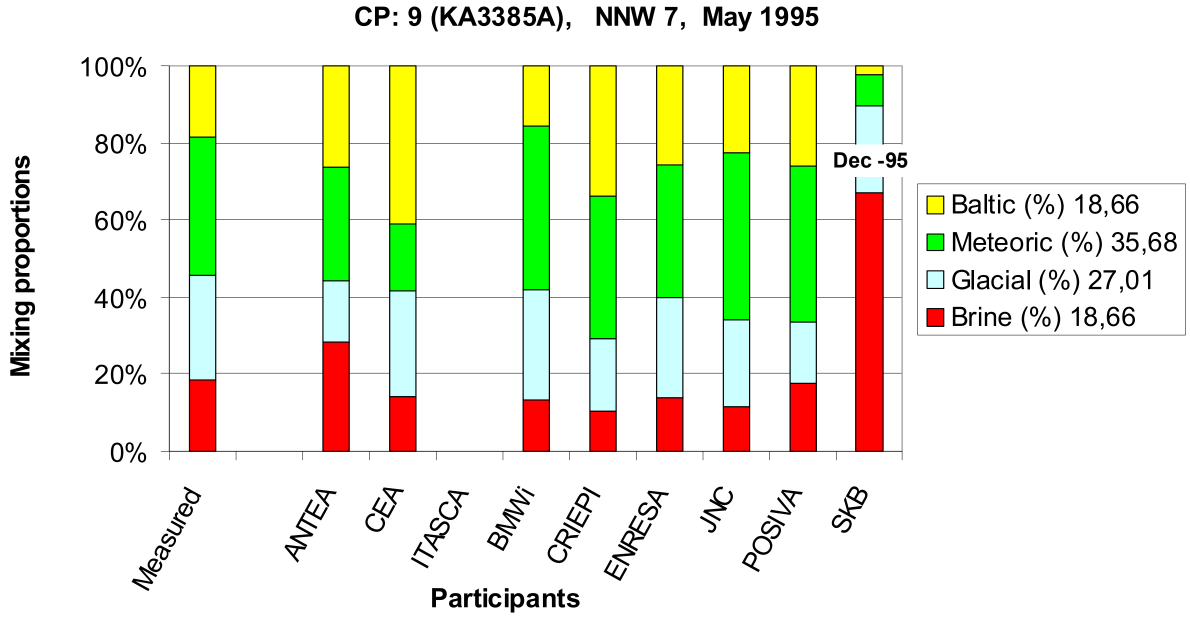


Task 5. Predictions of mixing proportions





Task 5. Predictions of mixing proportions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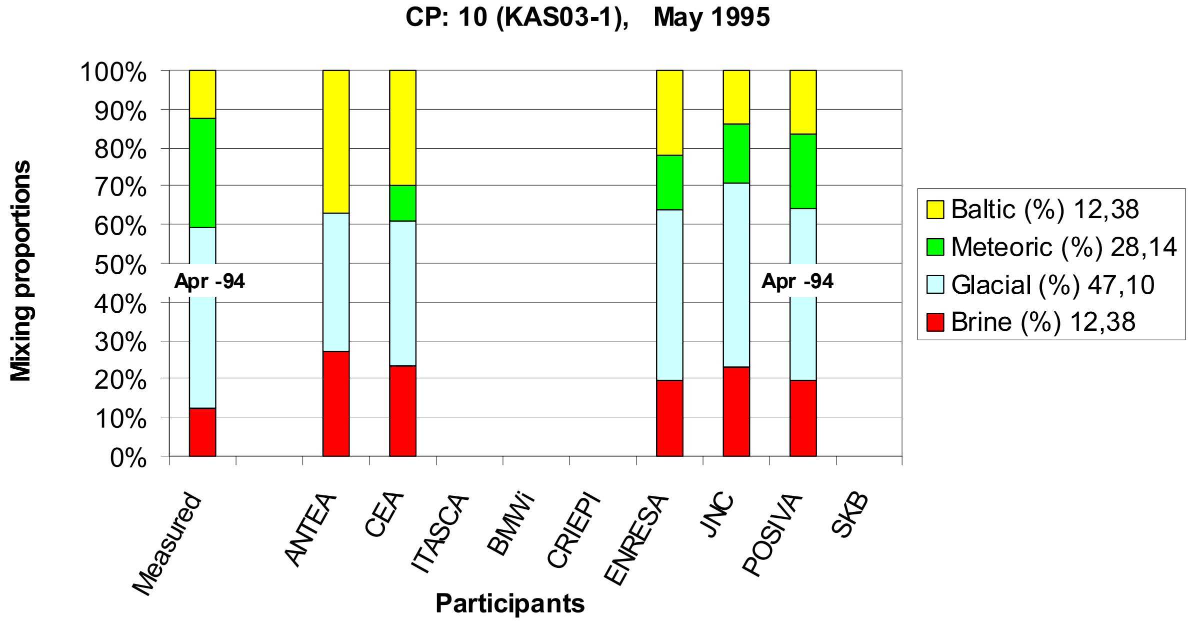
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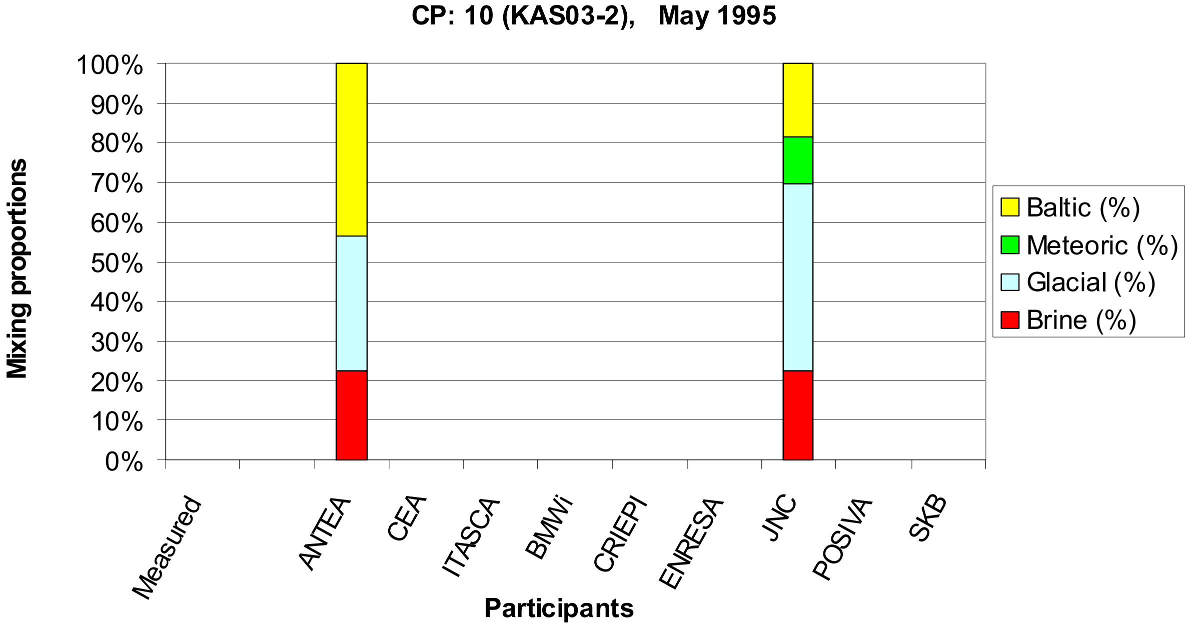
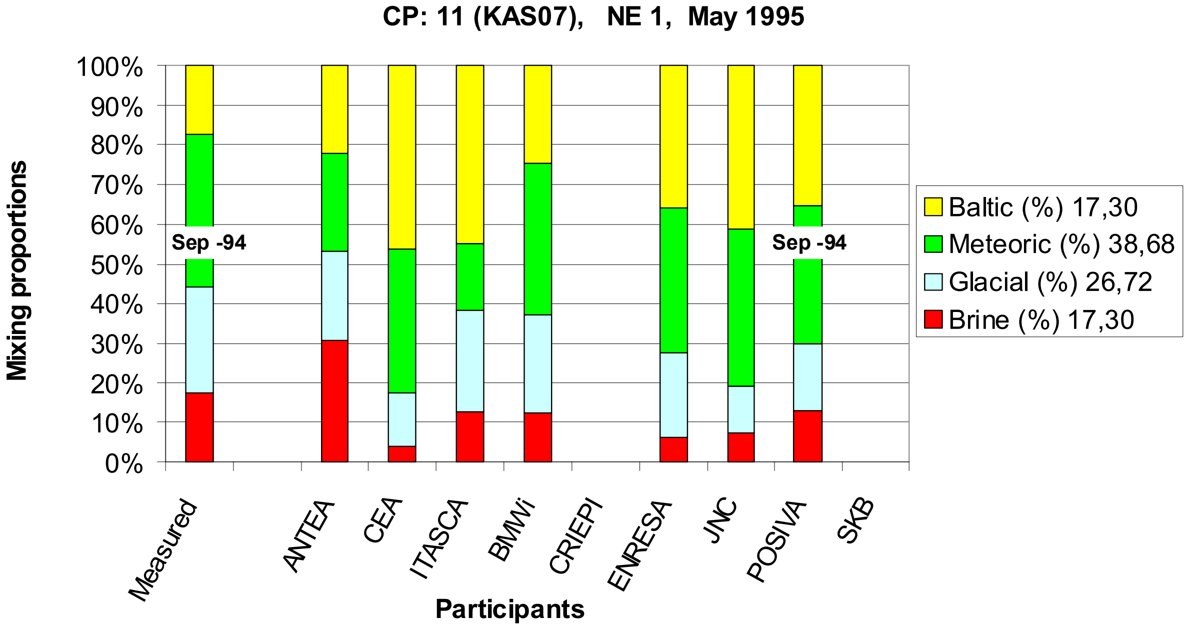
Task 5. Predictions of mixing proportions





Task 5. Predictions of mixing proportions