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Äspö Hard Rock Laboratory

Task Force on modelling of groundwater flow and transport of solutes

Review of Task 5

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February 2002

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Abstract

There are potentially considerable benefits in integrating geochemical information with models of groundwater flow. This can improve understanding, lead to more realistic models and improve confidence in the models. Task 5 of the Äspö Groundwater Modelling Task Force was set up to address the issues involved in such integrated modelling using the hydrogeological and geochemical data obtained during the construction of the underground Hard Rock Laboratory at Äspö.

In Part 1 of this report, we present a review of the work undertaken by the nine groups who participated in Task 5. We summarise what we consider to be the key aspects of their work and comment on issues specific to each group. We also comment on general issues, including the limitations of the numerical models for groundwater flow and solute transport used by the groups, issues related to the use of the Multivariate Mixing and Mass-balance (M3) approach for interpreting compositional variations in groundwaters which underpinned much of the work, the methods used for calibration and uncertainties.

Overall, we consider that Task 5 has been a significant advance on previous work. We do not know of any comparable study in terms of size of data set and complexity of flow system where such a broadly compelling use of geochemical constraints on a flow model has been achieved.

In Part 2, work to address a particular technical issue relating to the use of the M3 approach is discussed. The approach is based on interpreting the observed groundwater compositions in terms of mixing of a small number of reference groundwaters, with deviations from ideal mixing being interpreted as due to reactions. In much of the work using the M3 approach, it has been assumed that the mixing fractions obey the standard advection-dispersion equation, whereas in fact they do not. A study of the errors introduced as a result of this assumption has been undertaken. It was found that on average the errors were small, probably smaller than that resulting from errors in experimental measurements. However, in specific cases, the errors could be very large. This means that great care must be taken in inferring support for a groundwater flow and transport model on the basis of an apparent match between M3 mixing fractions predicted from groundwater transport modelling and M3 mixing fractions interpreted from measured groundwater compositions.

Sammanfattning

Det finns potentiellt sett avsevärda fördelar med att integrera geokemisk information med grundvattenflödesmodeller. Detta kan öka förståelsen, leda till mer realistiska modeller samt förbättra förtroendet för modellerna. Huvudsyftet för Task 5 arbetet inom Äspö Groundwater Modelling Task Force har varit att studera frågeställningar som uppstår vid integrerad modellering vid användning av såväl hydrogeologisk som geokemisk information. Använda data har inhämtats under byggandet av Äspö Hard Rock Laboratory.

I denna rapports Del 1 presenterar vi en summering av det hittills nedlagda arbete som de nio arbetsgrupperna inom Task 5 projektet har genomfört. Vi summerar det vi bedömer vara nyckelaspekterna av deras arbete och kommenterar specifika frågor för varje arbetsgrupp. Vi ger även generella kommentarer, inkluderande de numeriska modellernas begränsningar vad avser grundvattenflöde och transport av lösta ämnen. Dessutom kommenteras frågor i relation till användandet av ”Multivariate Mixing and Mass-balance (M3)” metodiken för tolkningen av vattenkemivariationer i grundvatten som ligger till grund för mycket av det utförda arbetet samt använda metoder för kalibrering och osäkerheter.

Sammantaget bedömer vi att arbetet inom Task 5 har gett avsevärda framsteg jämfört med tidigare arbeten. Vi känner inte till någon motsvarande studie vad gäller omfattning på använda data och flödessystemets komplexitet där i stora drag en övetrygande användning av geokemiska begränsningar på en flödesmodell har blivit uppnådda.

I Del 2 diskuteras en specifik teknisk fråga vad gäller användningen av M3-angreppssättet. Denna metodik baseras på tolkningen av observerade grundvattensammansättningar i termer av blandning av ett mindre antal av referensgrundvattenprov. En förändring i förhållande till fullständigmixning tolkas som orsakade av reaktioner. I mycket av arbetet med M3-angreppssättet har det antagits att blandningskomponenterna följer den standardiserade advektions-dispersionsekvationen, vilket i praktiken inte sker. En felanalys av detta antagande har gjorts. Denna visar att felen var i genomsnitt små, troligen mindre än felen vid de experimentella mätningarna. Dock, visar studien, att felen i specifika fall kan vara mycket stora. Detta betyder att stor varsamhet måste iakttas vid sökande av stöd för en grundvattenflödes- och transportmodell på basis av en uppenbar matchning mellan M3 blandningskomponenter beräknade från grundvattentransport-modellering och M3 blandfraktioner tolkade från uppmätta grundvattensammansättningar.

Executive Summary

Various countries are considering the disposal of radioactive waste in underground repositories constructed at depth in stable rock formations. Although the radioactive waste inventories and the design of the waste packaging vary from country to country, in all cases, the groundwater system at a candidate site is a very important factor affecting the safety of geological disposal. The chemical composition of the groundwater and its flow rate will affect the rate of corrosion of waste canisters and packages, and thus will influence the time that the waste remains totally contained, and will subsequently influence the rate of degradation of waste forms and rate of release of radionuclides. The directions and rates of groundwater flow also determine the potential pathways for radionuclide migration, and the rates of radionuclide movement away from a repository. Models of the groundwater composition and flow therefore play an important role in assessing the performance of a potential repository.

There are potentially considerable benefits in integrating geochemical information with models of groundwater flow and transport at a site (such as would be required in a repository performance assessment). The use of information on the variations of groundwater compositions in the development of the flow and transport models:

- can improve understanding of the flow system;
- has the potential to lead to more realistic and more robust models;
- is likely to improve confidence in the models.

However, there may be difficulties in integrating geochemical information into hydrogeological models. The relevant geochemical information consists of measured concentrations for various groundwater constituents at various locations. The concentrations are the results of mixing and reactions between the groundwater and the rocks through which it passes and between different groundwaters. The resulting patterns in the distribution of the different constituents may be complex and difficult to interpret. Further, it may not be easy to present the information in a readily understandable form.Task 5 of the Äspö Groundwater Modelling Task Force was set up to address the issues involved in integrating geochemical information with hydrogeological information, using the groundwater data obtained before and during the construction of the underground Hard Rock Laboratory (HRL) at Äspö in Sweden.

Nine modelling groups worked on Task 5. In the first part of this report, we present a review of the work carried out. The review is based primarily on the final reports produced by the participating groups. We summarise what we consider to be the key aspects of their work, and we comment on issues specific to the work of each group. A more detailed and comprehensive summary of the methods and assumptions, model geometries, input data and results is provided in the Summary Report for Task 5 (Rhén and Smellie, 2003). Our review comments cover both issues of detail in how the modelling was carried out and broader issues concerning strategies for model calibration and testing, for example:

- the conceptual and numerical models;
- uncertainties in the initial conditions;
- issues related to the use of the Multivariate Mixing and Mass-balance (M3) approach, which underpinned much of the work on the task;
- the approaches adopted for model calibration and testing;
- overall uncertainties including the possibilities of alternative models and the objectivity with which model outputs have been compared with observed data;
- the presentation of the final reports.

The groundwater flow and transport models developed by the groups were all based on the same underlying conceptual model. This resulted from the very extensive site investigations carried out at Äspö and from interpretative work outside Task 5, principally Rhén et al (1997a,b,c). In this model, groundwater flow is predominantly through Hydraulic Conductor Domains (HCDs), with weaker flows through the Hydraulic Rock-mass Domains (HRDs) between the HCDs. A wide range of numerical models were used in Task 5 to represent this model, encompassing continuum porous medium models, fracture-network models and pipe-network models, with some models having aspects of more than one of these categories. We consider that all of the models developed provide reasonable approximations, although some are more realistic than others.

One of the main findings of the groups was the sensitivity of the transport modelling results to the initial conditions assumed for the spatial variation of groundwater compositions. These initial conditions were obtained by interpolation and extrapolation from a small number of measurements, and therefore are likely to have significant uncertainties.

Most of the work carried out in Task 5 was based on the use of the M3 approach for characterising groundwater composition. This approach is based on M3 groundwaters in terms of mixtures of a small number of reference waters. The reference waters have physical significance, i.e. they represent distinct present and past groundwater masses, and. They are determined by a combination of a statistical analysis and expert judgment. The approach incorporates a prescription for determining the fractions of a groundwater sample corresponding to the reference waters. However, if there are more than three reference waters, there is uncertainty about these estimated mixing fractions (which is 0.1 for the groundwaters at Äspö).

We consider that the M3 approach provides a good means of presenting geochemical information in a way that can readily be understood by non-specialists. However, we have reservations about its direct use in calculations and to test models. In particular, because of the additional uncertainty introduced by the approach, tests of a model by comparison of calculated mixing fractions with mixing fractions determined from experimental measurements are less stringent and transparent than tests based on comparison of the measured concentrations of ionic solutes and isotopes. As a result one has less confidence in the model than would be the case if the test of the model were based on a direct comparison of predicted and measured concentrations of the groundwater constituents.

It was originally suggested that one possible approach for Task 5 would be as follows. A groundwater flow and transport model would be set up on the basis of the existing conceptual model and using existing values of hydrogeological parameters. The initial distribution of the groundwater composition, prior to construction of the HRL, would be estimated by interpolation and extrapolation from the measurements. The evolution of the groundwater compositions during the construction of the HRL would be predicted using the transport models and compared with observed compositions from borehole sections around the HRL. This comparison would provide an extra check on the model, beyond that provided by hydraulic observations alone. It might then be possible to modify the initial distribution of groundwater composition to obtain an improved model.

All of the participating groups calibrated the flow models against measured heads in boreholes and/or measured inflows to the HRL tunnel. Some groups then progressed to establish a solute transport model which was calibrated and tested against the geochemical data. The parameters obtained by the groups for the flow and transport properties of the system varied widely. Overall the approach seemed to be one of seeking the best model at each stage. However, we think that it might be better to try to determine the range of models that give an acceptable match to observations. In this way, the benefits of using the geochemical data could be quantified.

The final models obtained by all of the groups were described as giving good (or at least reasonable) matches to observations. However, we hesitate to describe any of the fits as good. We think that over-optimistic descriptions of the match of models to data detract from the achievements of the teams.

The presentation of the final reports could generally be improved. The techniques used are not always clearly explained. Standardisation of how model outputs and parameters were compiled would have made intercomparison much easier. The Summary Report has, however, achieved much in this respect (Rhén and Smellie, 2003).

Finally in Part 1 of this report, we present our view on the overall progress that has been made in integration of geochemical information into hydrogeological models. The objective is not an easy one because hydrogeological and geochemical data have different natures and have different significance for a flow and transport model. However, we consider that Task 5 has been a significant advance. The exercise has identified much more clearly than previously realistic aims for integrating geochemical information with hydrogeological modelling. We do not know of any comparable study, in terms of size of data set and complexity of both flow system and perturbing process, where such a broadly compelling use of geochemical constraints on a flow model has been achieved. There can be no doubt that, given hydraulic and geochemical conditions that are favourable to this type of exercise, the general objective of 'coupling geochemistry and transport modelling' will have an important rôle in future site investigations. In order to use geochemical information to test models, as in Task 5, appropriate data are needed. As well as data from boreholes within a site, data from regional boreholes would be necessary to adequately define the boundary conditions.

In Part 2 of the report, work to address a particular technical issue relating to the use of the M3 approach is discussed. In the work for Task 5, it was assumed that the M3 mixing fractions obey the standard advection–dispersion equation (ADE). This is the equation that is obeyed by the concentrations of the groundwater constituents, in the absence of reactions. However, if there are more than three reference waters, the mixing fractions do not actually obey the standard ADE, but a slightly modified equation containing an additional term, which does not have the form of any of the usual terms in the ADE. This is because the relation between the mixing fractions and the concentrations of the groundwater constituents is non-linear if there are more than three reference waters.

Therefore, use of the standard ADE for the mixing fractions will have introduced errors into the modelling. This issue is particularly important because the M3 approach may also be used in work to be carried out for the sites in Sweden chosen for investigation as potential candidate sites for a deep repository for radioactive waste.

A study of the issue was undertaken. The approach adopted was to consider various cases in which flowing groundwaters of different compositions mix and to compare mixing fractions calculated on the assumption that they obey the standard ADE with mixing fractions calculated from the transport equation that they really satisfy. The latter mixing fractions were actually determined by calculating the evolution of the groundwater constituents, which obey the standard ADE and then evaluating the mixing fractions, rather than by directly calculating the evolution of the mixing fractions using the equation that they satisfy. The calculations were carried out for cases in which there are simple analytical solutions to the standard ADE. This allowed the study to be carried out using a simple spreadsheet, rather than requiring the use of a finite-difference or finite-element program to carry out the transport calculations. In order that the study was as relevant as possible to the work undertaken for Task 5, the calculations were carried out for the relationship between the concentrations of the groundwater constituents and the mixing fractions used in the M3 analysis that underpinned most of the work on Task 5.

Both deterministic and probabilistic studies were carried out. It was found that, although the mixing fractions do not actually obey the standard ADE, the error resulting from assuming that they do is, on average, very small, and probably smaller than the typical error resulting from experimental errors in the measurement of the concentrations of the groundwater constituents. Therefore, this study provides support for the use of the assumption that the mixing fractions obey the standard ADE as a reasonable approximation.

However, the error can be much larger in particular cases. It should also be noted that the initial direction in which a mixing fraction is predicted to change on passing through a mixing zone may be incorrectly predicted. On average this occurs for slightly less than one of the mixing fractions. This means that great care must be taken in inferring support for a model on the basis of a match between the predicted and observed directions of change, if the mixing fractions have been calculated using the assumption that they obey the standard ADE.

Although this study provides support for the use of the assumption that the M3 mixing fractions obey the standard ADE, it is suggested that it might be better to calculate the evolution of the first two principal components using the standard ADE, and then evaluate the mixing fractions from the principal components. This would be both computationally cheaper and more defensible (because the principal components satisfy the standard ADE in the absence of reactions and sorption). It is considered that this approach is less likely to be viewed with suspicion by those not familiar with the M3 approach. It is considered that it might be undesirable to adopt an approach that might be considered questionable in work undertaken in support of a repository performance assessment, in particular.

In the case in which reactions, or sorption are not neglected, the only justifiable approach is to calculate the concentrations of the groundwater constituents from the transport equations that they satisfy, with appropriate sorption or reaction terms. This approach may also be a suitable approach in the case in which reactions and sorption can be neglected. The approach would, of course, be rigorous in such cases, and it would be an approach expected by hydrogeologists and geochemists unfamiliar with the M3 approach. As such it would be unlikely to be viewed with suspicion. However, the approach has a greater computational cost than either of the alternatives: making the calculations on the basis of the assumption that the mixing fractions obey the standard ADE, or determining the first two principal components using the standard ADE.

Finally, it should be emphasised that the use of the M3 mixing fractions to present geochemical information has considerable benefits in terms of presenting the information in a readily understandable form to those who are not geochemists. It is therefore recommended that whatever approach is adopted for modelling the mixing of groundwaters, the results are presented using the M3 mixing fractions.

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Part 1:

Coupling Geochemistry and Transport

A H Bath and C P Jackson

1. Introduction

Various countries are considering the geological disposal of radioactive waste in underground repositories constructed at depth in stable rock formations. Radioactive waste inventories for the repositories vary from country to country, comprising varying proportions of spent fuel, other high-level wastes, and intermediate-level wastes. The design of the packaging for the wastes similarly varies. However, in all cases, the nature of the groundwater system at a candidate site is an important factor affecting the safety of geological disposal. The chemical composition of the groundwater and its flow rate will affect the rate of corrosion of waste canisters and packages, and thus will influence the time that the waste remains contained; and will subsequently influence the rate of degradation of waste forms and rate of release of radionuclides. The directions and rates of groundwater flow also determine the potential pathways and the rates of radionuclide movement away from a repository. Models of the groundwater composition and flow therefore play an important role in assessing the performance of a potential repository.

At Äspö, an underground ‘Hard Rock Laboratory’ (HRL) was constructed some years ago as a research facility to support the Swedish radioactive waste disposal programme. The aim was to assist in the development and testing of methods for characterising a site for a repository for radioactive waste, and in demonstrating the feasibility of safe disposal of waste in such a repository. The Äspö Groundwater Modelling Task Force was set up to provide a forum for the international organisations supporting the HRL to work collaboratively on conceptual and numerical modelling of groundwater flow and transport in fractured rock.

Groundwater flow models in general describe the movement of groundwater from recharge areas, through geological formations of interest, to discharge areas where the flow of groundwater intersects the ground surface. The flow is driven by gravity, and may be affected by variations in groundwater density if salinity and/or temperature variations exist. The same principles govern groundwater movement in both high permeability systems (i.e. aquifers) and low permeability systems, such as the fractured crystalline rocks that are the focus of interest in the present study.

Groundwaters may show changes of composition along flow paths, reflecting active mixing between different groundwater masses at present, or variations of recharge or flow conditions in the past (‘palaeohydrogeology’). Salinity tends to increase with depth, and relative amounts of ionic solutes may change laterally as well as with depth.Groundwater flow models may describe the variations in density, but do not generally describe the variations of specific components in groundwater composition. Although the patterns of groundwater composition could, in principle, be used to check the groundwater flow models, this is not usually done.

Geochemical models for groundwater compositions simulate the chemical reactions between minerals and groundwaters and within the water itself, in combination with physical mixing. They are used to explain or predict changes in groundwater composition. Usually the models are used in 'static mode', that is they simulate reactions and mixing within a well-mixed system that is either closed (i.e. nothing is entering or leaving the system) or is a well-constrained sequence of closed systems. This represents a simplification of the processes that happen in natural groundwater systems. Recently, methods have been researched and developed to combine numerical models of groundwater flow with geochemical reaction models. Such 'fully coupled' models are still at an early stage of development, partly because of the computing power required to carry out the calculations, and also because of the complexity of the inter-relationship of reaction and flow, with the evolution of the system controlled by many factors, such as reaction kinetics and dispersion.

As well as the use of geochemical models for simulating and understanding the evolution of the composition of a groundwater system, it is also possible (as indicated above) that the observed variations in groundwater composition can be used to constrain the range of possible groundwater flow models. It is important to understand the rationale for using geochemical data to constrain a flow model. It depends on being able to use the geochemistry to identify discrete groundwater volumes that have sufficiently distinct characteristics, and remain sufficiently distinct for the duration of the simulated or observed flows. In other words, changes in groundwater compositions that are caused by the flow system and timescale of interest should be distinguishable from compositional variations that originated in the prior history of the groundwater system.

There are potentially considerable benefits in integrating geochemical models with models of groundwater flow and transport at a site (such as would be required in a repository performance assessment). The use of geochemical information in the development of the flow and transport models:
- can improve understanding of the flow system;
- has the potential to lead to more realistic and more robust models;
- is likely to improve confidence in the models.

However, there may be difficulties in integrating geochemical information into hydrogeological models. Geochemical information consists of measured concentrations for various groundwater constituents at various locations. The concentrations are the results of mixing and reactions between groundwaters with different compositions and reactions between the groundwater and the rock through which it flows. The resulting patterns in the distribution of the different constituents may be complex and difficult to interpret. Further, it may not be easy to present the information in a readily understandable form. This would be very important for a repository performance assessment, which would probably subject to considerable scrutiny.

Task 5 was set up to explore the issues involved in integrating geochemical information with hydrogeological information. The approach in Task 5 was to use the hydrogeological and geochemical data from Äspö, specifically to use the data that represent the disturbance caused by excavation of the HRL tunnel. In setting out with the Task, the Äspö Groundwater Modelling Task Force had the benefit of three factors:

1. The existence of an exceptionally large set of hydrogeological and hydrochemical data for the Äspö HRL and its vicinity;
2. Previous modelling experience, for various length and time scales, of the flow pattern before and after construction of the HRL;
3. Development of the M3 approach for characterising groundwater compositions in simple terms.

The task here is rather different, in terms of timescale, initial and boundary conditions, and other constraints, from integrating hydrochemical data for an undisturbed groundwater system with a palaeohydrogeological model of past groundwater flows.

Nine modelling groups within the Äspö Task Force participated in Task 5. In this report, a review of the work undertaken on Task 5 is presented, with brief summaries of some the key features of the models used by each team. A comprehensive overview and comparison of the approaches, geometries and parameter sets adopted by the participating groups is provided in the Task 5 Summary Report (Rhén and Smellie, 2003) which should be referred to alongside this Review Report.

The structure of the report is as follows. In Section 2, Task 5 is outlined. Much of the work on Task 5 used the 'M3' (Multivariate, Mixing and Mass-balance) approach (Laaksoharju et al., 1999) to describe the geochemistry. This approach is outlined in Section 3. In Section 4, the work carried out by the various participating groups is summarised, and specific issues relating to the work of each group are discussed. In particular, the objectives of the individual groups, which, in some cases, were not as far-reaching as the overall objectives of Task 5, are set down. In Section 5, general issues relating to the work carried out on Task 5 are discussed. Finally, in Section 6, the overall progress in integrating geochemistry and hydrogeology that has been made as a result of Task 5 is summarised.

2. Organisation of Task 5

2.1 Objectives of Task 5

Task 5 specifically addressed the integration of geochemical and hydrogeological modelling. It was based around modelling (i) the flow of waters into the underground tunnel that forms the Hard Rock Laboratory, and (ii) the chemistry of the inflowing waters, using data obtained during the construction of the Hard Rock Laboratory.

The specific objectives of Task 5 were:

- 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;
- To develop a procedure for integration of hydrological and hydrochemical information which could be used for assessment of potential repository sites.

2.2 Approach and Input Data

The approach that the SKB modelling team originally proposed to use for Task 5 is illustrated in Figure 1-1. Hydrochemical data for the pre-excavation groundwater system at Äspö, interpreted using the M3 approach, in terms of mixtures of reference waters, were to be used together with data for groundwater heads to establish initial and boundary conditions for a flow model of the system. A structural model and ranges of hydraulic properties had already been established in the earlier modelling of the groundwater system at Äspö, based on investigations prior to tunnel construction (Rhén et al., 1997a,b,c). The flow model was then to be used to simulate inflows into the excavation and the compositions of these inflows and of groundwaters at various parts of the modelled domain. The simulated values would be compared with the set of observed values as a first consistency check on the model. Expert judgment and an interpolation/extrapolation tool would then be used to refine the estimates of initial and boundary chemical conditions prior to re-running the numerical models of flow and transport and re-assessing the consistency between modelled and measured values for inflows and groundwater compositions.

It was left open to each participating group to decide the approach to model construction, testing and possible modification that was practicable given the available data and resources. The groups used a variety of approaches (see Section 4 and Subsection 5.1), which generally involved calibrating a flow model as well as a transport model.

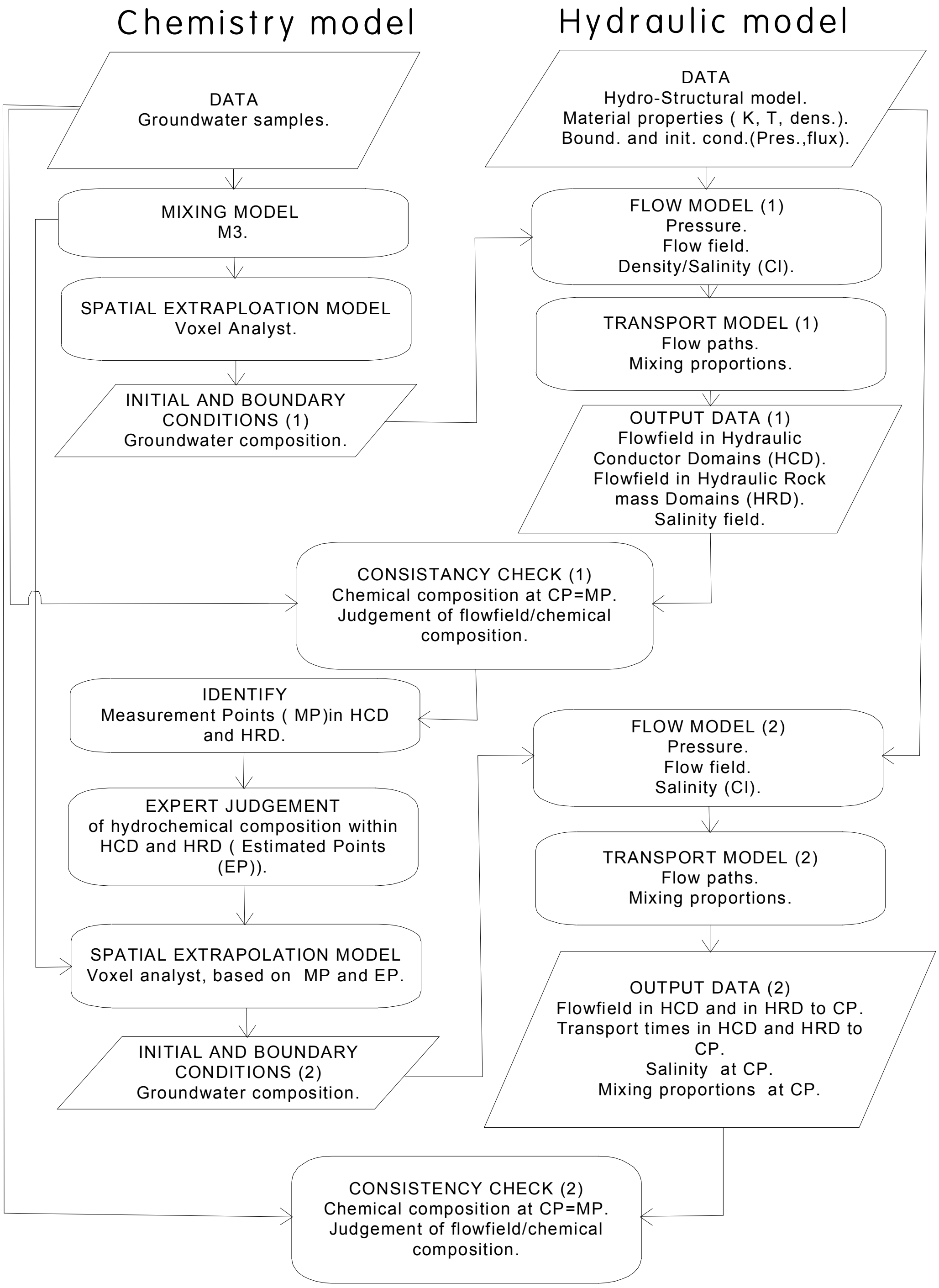


***Figure 1-1.** Flow diagram showing the proposed approach to integrating chemical information with the flow model for Task 5.*

The short title for Task 5, 'Coupling Geochemistry and Transport', is perhaps slightly misleading in that, in general, Task 5 did not actually address fully coupled modelling of groundwater flow and geochemical reactions. Only one of the groups (Enresa/UdC) used fully coupled modelling to simulate flow and reaction, restricting this to processes in a single fracture zone. Instead, Task 5 was an exercise in using the heterogeneous distribution of groundwater compositions to constrain the possible range of physical representations of groundwater movement in a transport model. The exercise is particularly workable for the transient groundwater flow system that is perturbed by the Äspö HRL because (a) the groundwater compositions vary naturally through the rock volume of interest, (b) the distribution of groundwater compositions prior to perturbation by the HRL is known to some extent, and (c) some compositional changes over time have been observed in inflows to the HRL.

The participating groups were supplied ‘data deliveries’ of structural/geometrical data, hydrogeological data and hydrochemical information (see Rhén and Smellie, 2003). The supplied structural/geometrical and hydrogeological data are basically those used in Task 3 modelling and were taken from Rhén et al. (1997c). The structural model comprises twenty-one Hydraulic Conductor Domains (HCDs). These are planar fracture zones with defined extents and with material properties derived from hydraulic testing with subsequent minor adjustment on the basis of numerical modelling. Mean measured transmissivities of these HCDs range from $3x10^{-4}$ to $1x10^{-7}$ m^2/s (Fig 5-13 in Rhén et al., 1997b). Thicknesses of HCDs are between 5 and 40 metres.

Most of the participating groups developed models that represented only the HCDs (or a subset of them; see Section 4). However, some groups developed models that also represented the Hydraulic Rock-mass Domains (HRDs) between the HCDs.

The hydrochemical information was provided in several forms. The basic ‘raw’ data, that is the concentrations of major solute ions and isotopes for the groundwater samples from the boreholes in the vicinity of Äspö and from inflows to the HRL, were supplied. These data had also been processed using the M3 approach (see Section 3 and Subsection 5.3), which interprets each groundwater sample as a mixture of reference waters, characterised by the fractions of the mixture corresponding to the reference waters. The participating groups could use either the raw data or the M3 mixing fractions, or both. Some of the groups also developed additional approaches to interpretation of the raw data to aid integration with the flow model.

Hydrochemical data and the resulting M3 mixing fractions were only available at a small number of sampling locations in boreholes and the HRL (although the data set is large compared to that for most site investigations). However, the solute transport models used by the participating groups require the initial composition of the groundwater throughout the domains modelled. In fact, as will be seen from the discussions in Sections 4 and 5, the results obtained by the groups were quite sensitive to the assumed initial conditions. Therefore, hydrochemical data (raw data and M3 mixing fractions) were interpolated and extrapolated to a rectangular grid using the program Voxel Analyst (which uses a method based on kriging) and the interpolated/extrapolated data were also supplied to the groups.

The data supplied to the groups also included the monitored inflows at a number of measurement points (‘MP’ in Figure 1-1), which are located at <2900 m along the tunnel. Fluxes and compositions of inflows corresponding to specific HCDs (i.e. at ‘EPs’ or estimation points in Figure 1-1) were interpolated from the MP data and provided data for calibrating the models. The models could then be used to calculate the inflows and their compositions at a number of control points (‘CPs’) for ‘blind test’ comparison with measurements.

In the approach originally proposed by SKB (see Figure 1-1), it was not anticipated that either the geometrical/structural model of the system or the hydraulic properties would be revised or calibrated during the exercise. The recommended hydrodynamic parameters, having come from the prior SKB modelling exercise reported by Rhén et al. (1997c), could be thought to be an adequate description of the system. The approach in Figure 1-1 appears to have been focused on revising the initial and boundary water compositions.

The modelling groups all used models based on the geometrical/structural model of Rhén et al. (1997c), although in a few cases minor changes to this model were made. The initial parameterisations of the models were based on the hydrogeological data in Rhén et al. (1997c), but all groups recalibrated the flow model using heads (and inflows also in some cases). For the majority of the modelling exercises, the calibration/testing procedure was slightly different to that illustrated in Figure 1-1. The flow model was calibrated against measured inflows and heads. Different adjustments of geometry, parameters and initial/boundary conditions were made by the various participants. Most of the modelling groups used the recalibrated flow model with the given boundary/initial conditions to calculate the compositions at MPs and CPs, and stopped there (see Section 5.2). In a few cases some further work was carried out to integrate hydrochemical data with the transport model: either recalibration of the model or using alternative geochemical models to improve simulation of mixing with reaction.

2.3 Participating Groups

Nine modelling groups participated in Task 5. These groups, and the methods that they used were:

Japan Nuclear Cycle Development Institute, Japan/Golder Associates Inc. (hereafter JNC/Golder)
This group used the FracMan/MAFIC/PAWorks structural-flow-pathways-transport model and the BGS-PCA hydrochemical data statistical analysis approach.

Empresa Nacional de Residuos Radiactivos, S.A., Spain/University of La Coruña (hereafter ENRESA/UdC)
This group used the TRANMEF-3 fracture flow and transport model.

Svensk Kärnbränslehantering AB, Sweden/Computer-aided Fluid Engineering AB/Duke Engineering & Services/GeoPoint AB (hereafter SKB/CFE)
This group used the PHOENICS flow and transport finite-difference model and the M3 hydrochemical data analysis tool.

Posiva Oy/VTT Technical Research Centre - Building & Transport and Energy, Finland (hereafter Posiva/VTT)
This group used the FEFTRA flow and transport finite-element model and the PHREEQC2 hydrogeochemical mixing and reaction model.

Central Research Institute of Electric Power Industry, Japan (hereafter CRIEPI)
This group used the FEGM-B flow and transport finite-element model.

Agence Nationale pour la Gestion des Déchets Radioactif, France/ITASCA (hereafter ANDRA/ITASCA
This group used the 3-FLO interconnected pipes model for flow and transport.

Agence Nationale pour la Gestion des Déchets Radioactif, France/Commissariat à l'Energie Atomique-DMT (hereafter ANDRA/CEA)
This group used the CASTEM2000 fluid mechanics model for flow and transport.

Agence Nationale pour la Gestion des Déchets Radioactif, France/ANTEA (hereafter ANDRA/ANTEA
This group used the TAFFETAS mixed hybrid finite-element dual-porosity model for flow and transport.

Bundesministerium für Wirtschaft und Technologie/Bundesanstalt für Geowissenschaften und Rohstoffe, Germany (hereafter BMWi/BGR)
This group used models from the DURST/Rockflow suite of finite-element models. SM2 was used for dual-porosity flow and TM2 was used for transport. PHREEQC2 was used for modelling hydrochemical mixing and reaction.

Each participant implemented a modelling approach appropriate to the capability of the computer codes and resources available to them. Task 5 was not intended as an inter-comparison of models, but as an exercise in the development and evaluation of an overall approach to the integration of geochemical information with hydrogeology. However, inevitably some aspects of the results relate to differences between the codes and approaches used by the different groups. For example, some codes included capabilities for particle–tracking calculations (see Section 4), which enable flow paths and travel times to be obtained, whereas other codes did not have such capabilities.

Hydrochemical data that had already been interpreted as mixing fractions using the M3 approach were used by all the groups. The M3 approach is described in Section 3. Some of the groups (see Section 4) also used alternatives to this approach.

2.4 Organisation of the Review

The input data sets that were made available to each participating organisation, the details of the modelling approaches and parameters adopted by each group, and the output results have been compiled in the Task 5 Summary Report (Rhén and Smellie, 2003). This review and evaluation has been based mostly on the individual task reports of the participants (Wendling, 2000; Grenier and Benet, 2000; Billaux and Paris, 2001; Liedtke and Klennert, 2001; Hasegawa et al., 2001; Molinero et al., 2001; Dershowitz et al, 2001; Luukkonen and Kattilakoski, 2001; Svensson et al., 2002), and was prepared in parallel with the preparation of the Summary Report.

Initial comments from the reviewers were presented to the participants at the 13th Task Force Meeting in Carlsbad, USA (February 2000; A Bath only) and the 14th Task Force Meeting in Gothenburg, Sweden (November 2000). Subsequently, in January 2001, the reviewers delivered preliminary review comments and suggestions for clarification of the draft versions of task reports to the participants. These comments were taken into account in the preparation of final versions of the reports. This report therefore focuses mostly on more general comments on the methodologies, interpretations and overall significance of Task 5.

The reviewers wish to acknowledge the contribution to their task made by many discussions with the participating modellers in which methods have been explained and misunderstandings clarified. The participants represent some of the leading groups working on groundwater flow, radionuclide transport and repository safety. It is an outstanding achievement to have brought them together in Task 5 of the Äspö Groundwater Modelling Task Force, for which the foresight of their sponsoring organisations should be duly acknowledged. Comparative exercises such as this are invaluable for making objective progress in this type of science. The reviewers also acknowledge the central role of SKB and its staff and local consultants, especially the SKB Project Manager (Peter Wikberg), the Task Managers (Ingvar Rhén of VBB Viak AB and John Smellie of Conterra AB) and the M3 consultant (Marcus Laaksoharju of GeoPoint AB). The views expressed in this report are those of the individual reviewers and do not necessarily represent the views of SKB or of any particular organisation that has been involved in Task 5.

3. The M3 Approach

An important aspect of the integration of hydrogeology and geochemistry is the approach adopted for characterising volumes of groundwater. As indicated in the Introduction, most of the work on Task 5 was based on the use of the Multivariate Mixing and Mass balance calculations (M3) approach (Laaksoharju et. al., 1999a). This is a technique that characterises groundwater compositions in a way that may be readily understandable by non-specialists.

The approach is based on describing groundwater compositions in terms of mixtures of a small number of reference waters. The deviations of groundwater chemistry from the results of ideal mixing are interpreted as the results of reactions. In addition to its use in interpreting geochemistry at Äspö (Laaksoharju et al., 1999b), M3 has also been used for interpreting groundwater compositions in the Oklo natural analogue study (Gurban et al., 2000) and has also been demonstrated with the data set from Whiteshell Research Area, Canada (Laaksoharju et al., 2000).

The M3 approach consists of four main steps. The first step is a principal component analysis of the measured compositions of the groundwater samples. Principal component analysis is a standard technique of multi-variate analysis. If the composition of each sample (i.e. data for the major solutes Cl, Ca, Na, Mg, K, SO_4 and HCO_3 together with the isotopes δ^2H, δ^{18}O and ^{3}H) is taken to correspond to a point in a multi-dimensional space with a coordinate for each constituent, principal component analysis consists essentially of seeking a rotation of the coordinates to determine new coordinate axes (directions of principal components) such that the spread of the projection of the cloud of points corresponding to the samples onto the first new axis is as large as possible; and given this, the spread of the projection onto the second new axis is as large as possible, and so on (see Figure 1-2). The principal component analysis is actually carried out in terms of standardised values, $\hat{c}_\alpha$, of the measurements of the concentration of the different groundwater constituents, which are given by

$$\hat{c}_\alpha = \frac{c_\alpha - m_\alpha}{s_\alpha} \quad , \tag{1}$$

where

c_α is the concentration of the α'th groundwater constituent;
m_α is the mean of the measurements of c_α;
s_α is the standard deviation of the measurements of c_α.

The use of standardised values enables quantities that have different units or different orders of magnitude to be taken into account in the analysis on the same footing. The principal components, P_α, are linear combinations of the standardised concentrations of the groundwater constituents:

$$P_\alpha = \sum_\beta a_{\alpha\beta} c_\beta \quad , \tag{2}$$

where $a_{\alpha\beta}$ are constant coefficients (called 'loadings' in principal component analysis).

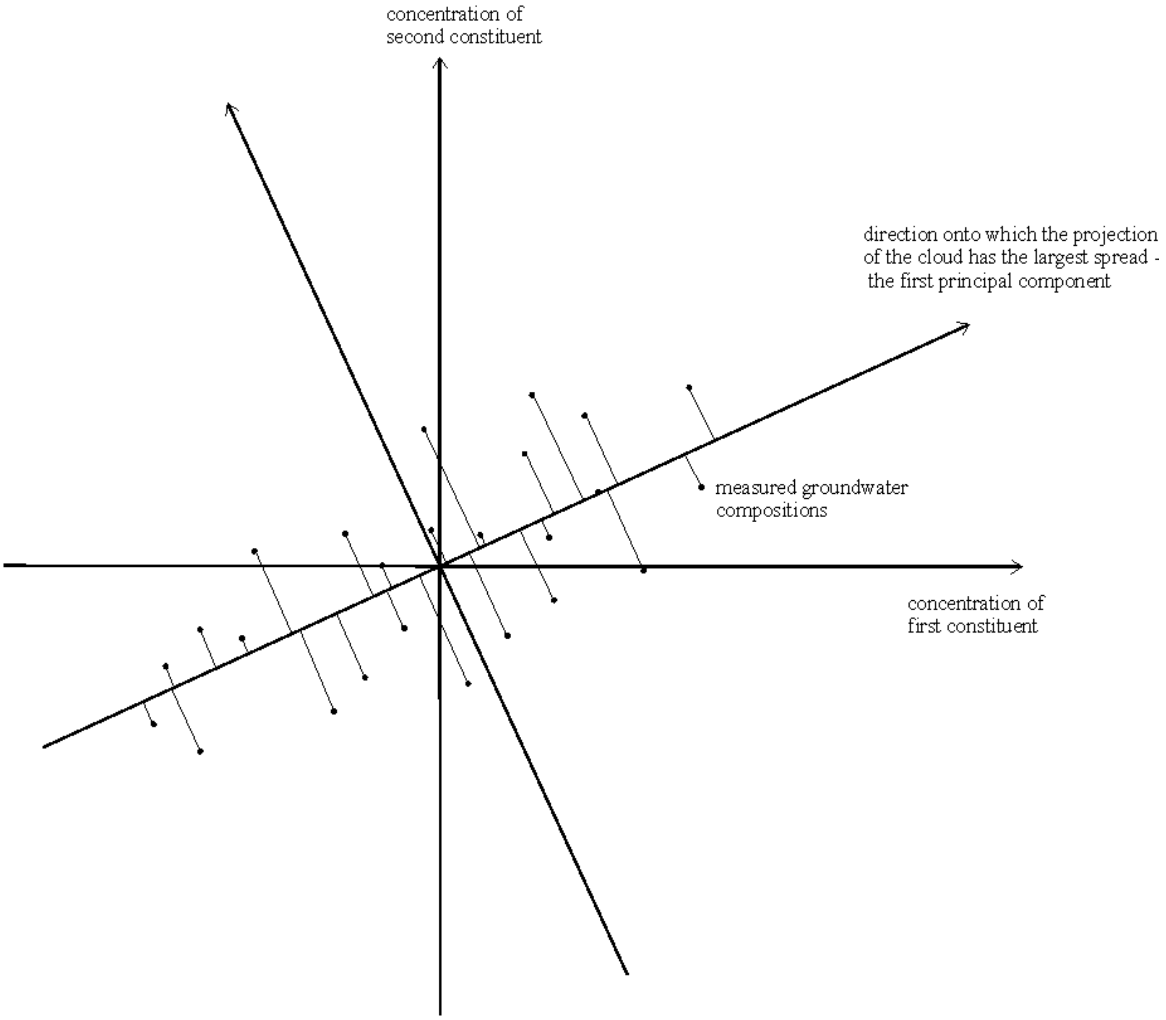


Figure 1-2. Illustration of the process of determination of principal components for a two-dimensional example.

In many cases of interest, the cloud of points only has a large spread in two (or perhaps three) orthogonal directions, that is, the new axes (each of which are particular linear combinations of the original groundwater constituents. Effectively the quantities corresponding to the remaining orthogonal directions are correlated with the quantities corresponding to the first two (or three) directions. In this case, the bulk of the information in the original measurements can be conveniently presented, without significant loss of information, in the projection of the cloud of points onto the first two (or three) new axes.

For clarity of presentation, the case in which two principal components are adequate to summarise the geochemical information will be discussed here. The modifications to deal with the case in which it is better to use three (or even more) principal components are straightforward. The projection of the scatter plot onto the first two principal components will be referred to as the 'M3 plot'.

The second step is to identify a small number of reference waters. This is done on the basis of the M3 plot, supported by physical and geochemical understanding of the groundwater flow system at the site of interest. The aims are that the points in the M3 plot corresponding to the reference waters should form the corners of a polygon, which contains all the points in the M3 plot corresponding to the observed groundwater compositions at the site, and that the reference waters should correspond to water compositions that have physical and geochemical significance for the site, taking into account the fact that all water compositions will subsequently be approximated as mixtures of the reference waters. The reference waters are not uniquely determined by the scatter plot, but depend, to some extent, on the judgment of the analyst.

The third step is to determine for each sample a mixture of the reference waters that would have the same proportions of the two principal components as the sample. If there are only three reference waters, then this can only be done in one way. In this case, the fraction of each reference water in the mixture is given by the ratio of the area of the triangle whose corners correspond to the two other reference waters and the sample to the area of the triangle whose corners correspond to the reference waters (see Figure 1-3, and the discussion in Laaksoharju et al., 1999a, where this is described in different, but equivalent, terms).

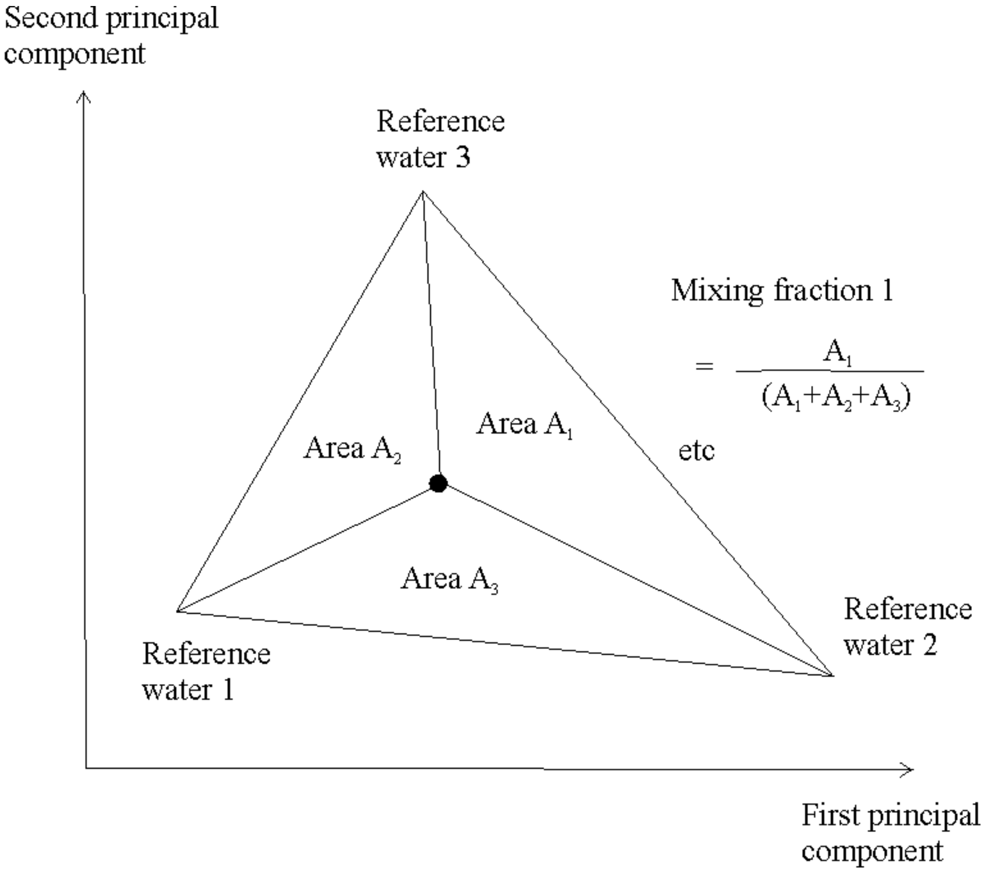


Figure 1-3. *The calculation of the mixing fractions for a case in which there are three reference waters.*

However, if there are more than three reference waters (in a case in which the analysis is being carried out on the basis of the first two principal components), then the mixing fractions are not uniquely determined. For example, if there are four reference waters, the point at the intersections of the lines between the pairs of points corresponding to the reference waters that are diagonally opposite one another in the M3 plot could be expressed as a mixture of one of the two pairs of diagonally opposite reference waters, or as mixture of the other pair of reference waters, or as various mixtures of all four reference waters.

In order to deal with this potential ambiguity, a definite prescription for determining the mixing fractions is given as part of the M3 methodology. The point in the M3 plot corresponding to a mixture of the reference waters in equal proportions is determined. The polygon formed by the points corresponding to the reference waters is subdivided into triangles by lines joining the corners to the central point. Then, the mixing fractions for a particular sample are determined as follows. The triangle in which the point in the M3 plot corresponding to the sample lies is determined. Fractions of the three corner waters (two reference waters and a mixed water corresponding to the central point) that would give a mixture with the same first two principal components as the sample are determined using the prescription for three reference waters described above. Finally, the mixing fractions for the original reference waters are calculated. This gives a unique prescription for the mixing fractions. In order to recognise the ambiguity, a prescription for the uncertainty in the mixing fractions is also given. For the groundwaters at Äspö, the uncertainty was estimated to be ±0.1, and it was also stated that mixing fractions of less than 0.1 have no significance (Laaksoharju et al., 1999b).

The fourth step is to determine, for each groundwater sample, the deviations of the concentrations of the various groundwater constituents from the values that they would have as a result of mixing the reference waters in the fractions given by the calculated mixing fractions. These deviations are interpreted as the result of reactions.

4. The Work of the Groups

In this Section, we summarise what we consider to be the key aspects of the modelling undertaken by each of the participating groups as described in their final reports, and we discuss issues specific to the work of each group. General issues, common to the work of all the groups, are discussed in Sections 5 and 6. This chapter should be read alongside the Summary Report, which gives comprehensive details of modelling approaches and parameters used by each of the groups (Rhén and Smellie, 2003).

4.1 ANDRA/ANTEA (Wendling, 2000)

4.1.1 Key Points

The ANTEA group joined Task 5 some time after it had started, so they limited their work to the calibration of a pseudo-steady-state flow model against heads. That model was then used for a calculation of transient flow in which the four M3 reference waters were transported.

In their model, both the HCDs (‘fractures’) and the rock mass between these were represented. (This model was described by the group as a ‘dual-porosity’ model.) The fractures were approximated as planar features. Fractures deemed to have an insignificant effect were omitted and some of the fractures were combined. In particular, the EW-1S and EW-1N HCDs were represented by a single fracture with different permeabilities parallel and normal to the fracture. The effect of variations in density were neglected, on the basis that these would only lead to head variations of order a few metres, which is small compared to the head variations resulting from tunnel construction. The Mixed Hybrid Finite-Element (MHFE) method was used to carry out calculations. Fractures, which were all represented as 10m thick zones with appropriate permeability, were modelled as being two elements thick.

An initial calibration was carried out in which the permeabilities of the fractures and rock mass zones were adjusted to try to match the steady-state head distribution before tunnel construction and the quasi-steady head distribution in November 1993 (at the end of a period when work on the tunnel had stopped temporarily). Although the permeabilities that gave the best match generally differed considerably from their initial values, the values were generally in reasonable agreement with the values obtained by the group in earlier modelling work for Task 1, using a different model with different fractures.

On comparing calculated and measured M3 mixing fractions, the group found that neglecting the rock mass zones had little effect on the results. The rock mass zones were therefore omitted from subsequent modelling in order to reduce computational costs.

The group found that a Galerkin finite-element scheme gave different results to the MHFE scheme used. They also found that the results obtained were sensitive to the scheme used for interpolating measured heads and concentrations to the mesh used, with one possible scheme giving very different results. In view of the uncertainties associated with the M3 mixing fractions (see Subsection 5.3), the group examined the effect of adding a random ('white noise') error, with similar magnitude to the uncertainties associated with the M3 mixing fractions, to the data for the M3 mixing fractions.

The team carried out a study in which parameters and aspects of the model were varied one at a time to try to improve the match to observations. They found, surprisingly, that the use of hydrostatic boundary conditions rather than conditions obtained from the regional flow model developed by Svensson (1999) gave a better match. They also found that changes to the kinematic porosity, storage and dispersivity all improved the match to observations. They then combined all the changes that individually improved the model into a single model. They found that the average difference between calculated and measured mixing fractions was about 0.1, which is similar to the uncertainty in M3 mixing fractions. The group therefore judged that the match to observations was satisfactory.

4.1.2 Comments

The ANTEA group judged that the fit to observations was acceptable on the basis that the average difference between measured and modelled mixing fractions was similar to the uncertainty of 0.1 in M3 mixing fractions. However, this view does not appear to have taken statistical considerations properly into account. It would appear that the average difference is sufficiently larger than its expected value that the difference is statistically significant.

The transient transport calculation was undertaken starting from the (nearly) steady-state flow field in November 1993 (i.e. 3 years after the start of tunnel construction). However, it seems that the initial distributions of the M3 mixing fractions for this calculation were the distributions prior to tunnel construction. The concentration distributions would have changed during the initial period of tunnel construction, and would have continued to evolve even during the period when the flow is almost steady. The significance of this mismatch in the model calibration is not discussed.

It appears that the model may have been calibrated to give a match (for the nearly steady-state flow model) to the observed water table in November 1993, and possibly also (for a modified version of the model) to the observed water table before tunnel construction. But there is no discussion of the criteria for the match, and of the extent to which modelled and measured head differences have been minimised. Calibration of the model did not take into account the data for the evolution of the heads at the measurement locations and the tunnel inflows during the prior period from the start of tunnel construction up to November 1993. However, these data provide valuable information about the hydraulic properties of the HCDs and the rock between them. It also seems that the model has been calibrated with heads alone and not with inflow volumes after November 1993. This makes the sources of error in the modelled M3 fractions less easy to interpret, because they will depend on errors in flow rates and distribution as well as on boundary and initial hydrochemical conditions.

The model used, MHFE, has allowed the effect of storage in the rock mass between the HCDs (which is described as ‘matrix’, but see the discussion in Subsection 5.1) to be explored. The conclusion reached here is that ‘the rôle of the rock matrix [i.e. HRDs] is not predominant’, and for the bulk of the modelling it has been ignored, i.e. the model is a simple network of interconnected fractures. This conclusion is rather opposed to conclusions of other groups (e.g. Golder/JNC, see Subsection 4.7, and SKB/CFE, see Subsection 4.9), but may be logical in terms of the short timescale of the transient flow experiment being modelled. Storativity and kinetic storage for the fractures were increased by an order of magnitude, which may also be a compensating factor.

The sensitivity analyses for specific storage of fractures do not really justify the statement that ‘a higher specific storage gives better results’. The poor matches between data and simulations seem to depend on factors other than storativity, so the sensitivity analysis is not very meaningful. In view of this problem, it is difficult to see that much can be learned about sensitivity to fracture storage.

An interesting attempt has been made to quantify the effect of the uncertainty in M3 values, which is quoted as being about ±0.1. This was done by introducing a ‘white noise’ of 0.1 in the M3 data, presumably by adding independent random contributions drawn from a suitable normal distribution to the M3 fractions at each voxel (in the rectangular grid to which the initial conditions were interpolated). However, these values are not independent but depend on the values of the M3 mixing fractions for the actual groundwater samples. Therefore, taking the errors in the M3 mixing fractions for each voxel to be independent is not a very good representation of the uncertainty. This would mean that the uncertainties in nearby voxels would be uncorrelated and would probably be averaged out over a travel path, whereas the uncertainties should be correlated, and might well not be averaged at all over some paths. Therefore, the statement that ‘the relatively high uncertainty on M3 concentration is causing no significant bias in the results’ is not justified by the results presented in the report, although it may be true.

The results of the study of the effects of uncertainties in M3 concentrations were used to support the use of boundary conditions that do not change with time. The argument presented may not be justified. The analysis undertaken examined the effects of uncorrelated random changes to the M3 mixing fractions. However, it would be expected that the changes to the boundary conditions would exhibit correlation over considerable distances. It is therefore not appropriate to make inferences about the effect of such changes from the effects of ‘white noise’. In particular, it would not be expected that the changes due to the evolving boundary conditions would necessarily average out over travel paths.

It is stated that ‘from a theoretical point of view MHFE method is "better" to determine velocity fields and transport calculations. Therefore, calibrated parameter values determined by this method should be preferred.’ This statement may not be entirely justified. The MHFE leads to velocity fields that are more physical, in terms of local mass balance (as indicated by ANTEA). However, for a given problem and discretisation into finite elements, the error in the calculated head is generally less for standard finite elements than for the MHFE method. Therefore, if a model is calibrated, at least partly against measured heads, the standard finite-element method may give more accurate parameters. If there are significant differences between the results obtained using the two approaches, it may be an indication that the numerical discretisation is not adequate.

It is stated that ‘in order to improve the results of the model it would be better to use hydrostatic pressure at 0 mASL for boundary conditions in heads’ (note: mASL is an abbreviation of metres above sea level). This could be misleading, although we note that there is a discussion of possible explanations for this ‘surprising result’. Even though using hydrostatic pressure of 0 mASL on the boundary gives (for the model used) a better match to observations than the boundary conditions originally used, it does not mean that the model would be better. The original boundary conditions are more realistic physically. In general, the fact that the match between calculated values calculated for a model and observations can be improved by taking one, or more, parameters to have unphysical values does not mean that the unphysical values are right. If anything, it suggests that some aspect of the model is not quite right.

4.2 ANDRA/CEA (Grenier and Benet, 2000)

4.2.1 Key Points

The ANDRA/CEA group saw Task 5 as providing a unique opportunity to test models against reality. However, they joined the Task some time after it had started, and the work that they were able to do was therefore limited.

In their model, only the HCDs were represented. These were modelled using 3D finite elements. A novel technique was used to handle the potential difficulties in setting up a grid in which the intersections of all the HCDs were represented. Rather than setting up an overall grid for the network of HCDs, an independent 3D grid for each HCD was set up, with consistency between the pressure and concentrations at the intersections ensured using a Lagrange multiplier technique. The tunnel, together with a skin representing the effects of grouting, was also included in the model.

In their flow calculations, the effects of groundwater density variations due to variations in salinity were taken into account. In order to reduce the computational resources required, most of the calibration of the model was carried out using a density that varied spatially, but remained constant in time. Then fully coupled calculations of flow and salinity transport were carried out to examine the effect of the transient variations in salinity. Calculations of the transport of M3 mixing fractions (treated as conservative tracers) were then carried out on the basis of the calibrated flow model. It was not practicable to calibrate the transport model in the time available.

Because of the approach used to represent the intersections of HCDs, it was not possible to carry out simple backward particle-tracking calculations. Instead, the group carried out backwards transport calculations (using the Lagrange multiplier approach to ensure consistency at intersections) and then estimated the travel time from the movement of the centre of the plume.

4.2.2 Comments

The use of the Lagrange multiplier technique to ensure continuity of the flow and transport variables at intersections of HCDs, as opposed to generating grids in which the elements all fit together, is very ingenious. It is not clear whether all intersections of HCDs were handled using the Lagrange multiplier technique, or just a few. Presumably this technique relates the effective properties of this artificial connectivity directly to the properties of the HCDs contributing to each intersection. How realistic and adaptable (i.e. for sensitivity analyses) this is could be important because these intersections have an important rôle in groundwater mixing. It seems to be as good a representation of HCD intersections as representations in other Task 5 models.

This model considered only the fracture network, without any intervening HRDs. The interplay between calibration of the fracture storativity, storage in the HRDs and connectivity at intersections could not be investigated. It is not clear what value was used for the transverse dispersion length, and what boundary conditions were imposed to represent the Baltic Sea bed.

Grouting has been allowed for in the model calibration, specifically for HCDs NE1 and NE3. It is said that this has lowered sensitivity to the transmissivity values for these HCDs, which anyway have the highest transmissivity values. It is not clear what has been changed to simulate grouting, and what parameters are assumed to be affected - just transmissivity values, or heads as well? It would be useful to compare how the model allowing for grouting compares with other models that have not allowed for grouting, but there is insufficient information to do this.

It is not clear whether the very short travel times presented (weeks to months) correspond to travel in the steady-state flow field after tunnel construction, to travel in the steady-state flow field before tunnel construction or to travel in the flow field during tunnel construction arriving at the control points at a specified date.

4.3 ANDRA/ITASCA (Billaux and Paris, 2001)

4.3.1 Key Points

The objective of the ANDRA/ITASCA group was to gain experience in modelling a real site and to examine the complexities introduced by considering geochemistry and hydrogeology at the same time.

In the ITASCA model, only the HCDs were represented. Each HCD was represented as a regular lattice of channels (with either a square grid or a square grid plus diagonals), together with channels along the intersections of HCDS. The conductivities of the channels for each HCD were chosen so that the HCD had a specified transmissivity. In addition, links were added between the EW-1N and EW-1S HCDs, which would otherwise not have been connected in the domain modelled. The tunnel was represented in terms of the inflows to its intersections with the HCDs.

The model was calibrated to the observed heads by adjusting the transmissivities of the HCDs. A small number of variants were considered and the best of these was chosen.

Then transport calculations were carried out for conservative species and for the M3 mixing fractions, which were treated as conservative tracers. A particle-tracking approach was used. The parameters of the model were further adjusted to try to achieve an acceptable match to the measured mixing fractions. Again, the best of a small number of variants was chosen. Then backward pathlines to various locations were calculated.

Coupled calculations of flow, transport and reaction were carried out. The calculations were carried out on a restricted sub-domain to reduce computational requirements. The approach used for the transport calculations was the Discrete Parcel Random Walk method whereby the velocity field is first solved, then initial chemical concentrations and 'source terms' (i.e. mineral phases) are introduced as a large number of particles to satisfy solute mass budgets. Each particle moves according to the velocity field, modified to include hydrodynamic dispersion by randomly sampling a Gaussian distribution related to the dispersion coefficient. At each time step, the geochemical reactions in each pipe are modelled to account for dissolution and precipitation. Electroneutrality is secured by adding a 'dummy' non-reactive charged component. Although transport of several solutes (Na^+, Ca^{2+}, CO_3^{2-}, Cl^-, SO_4^{2-}, Mg^{2+}, K^+, H^+) was modelled, $MgCO_3$ precipitation is the only two-phase reaction that could be simulated. The group point out that this is an implausible condition.

4.3.2 Comments

With the model used, 'dispersion' is controlled by the length of the channels, which effectively set a length scale for dispersion, analogous to the dispersion length. It would be of interest to examine the effect of changing the channel length (or equivalently channel density).

It is claimed that there is a good agreement between the calculated and measured heads. However, in Figure 2.9 of Billaux and Paris (2001), it appears that there are significant differences between calculated and measured heads for KAS02 section 346-799 and KAS03 section 377-532, for example. These discrepancies require some comment.

It is implied that the reason for changing from a proportional skin at the bottom of the Baltic Sea to a uniform skin is that the model overestimates the fraction of Baltic water arriving at the control points. However, it appears from the figures that, in the long term, the fraction of Baltic water is little changed however the skin is represented. This seems to be counter to the conclusions from other modelling.

It is interesting that dispersion in the model is dominated by mixing at intersections between HCDs. This points also to the potential significance of how the intersections are simulated with the Lagrange multiplier technique in the ANDRA/CEA model (see Subsection 4.1) rather than, perhaps, to the values given for transverse dispersivity. The issue of dispersion - how it is parameterised, and what are the indirect influences on it (e.g. how the initial conditions are set, how mixing at intersections is simulated, timescale whereby mixing rather than initial compositions along single fractures becomes more important as duration of flow increases, etc) requires careful consideration.

Although the coupled geochemical model approach is interesting, it is severely deficient in terms of realistic water-rock reactions, not the least problem being that only a $MgCO_3$ solid phase is included in the model. $MgCO_3$ is geochemically unrealistic in most natural conditions since $CaCO_3$ and dolomite [$CaMg(CO_3)_2$] are the relevant carbonate phases. The reality for Äspö groundwaters is that Mg is controlled by reactions with minerals other than carbonates. Therefore, the outputs from this attempt at geochemical modelling are not considered further here.

4.4 BMWi/BGR (Liedtke and Klennert, 2001)

4.4.1 Key Points

In the model developed by BGR, only the HCDs were represented. Initially, a model was considered in which only four of the HCDs (NE-1, EW-3, NE-2 and NNW-4) were represented. In the final model developed, which gave an improved match to the observed heads, ten HCDs were represented. The HCDs were represented using two-dimensional finite elements, with refinement in areas of particular interest, such as intersections with the tunnel. On most of the HCDs, the transmissivity was taken to be constant away from the tunnel. NE-2, NNW-4 and EW-3 were each subdivided into four parts with the same permeability, but different thickness, and therefore different transmissivity. Elements in the vicinity of intersections of an HCD with the tunnel were taken to have smaller transmissivity than the HCD. The tunnel itself was represented using one-dimensional elements. The initial and boundary conditions for groundwater head and M3 mixing fractions were obtained by interpolating (using nearest-neighbour interpolation) from the values on a grid of points that were supplied as part of the available data (see Subsection 2.2).

The model was first calibrated to match the inflows to the tunnel by adjusting the transmissivities of the HCDs. Then the storativities of the HCDs were adjusted to give a match to the observed transient heads. The match was considered to be reasonable, although the group noted that the calculated heads tended to be too low. Then transport properties were adjusted to try to match to the observed mixing fractions. The group note that, although the match to observations is good for some boreholes, for others the discrepancies are large (larger than the quoted level of uncertainty associated with M3 mixing fractions). They suggest that the discrepancies may be due to the use of poor initial conditions, which were obtained by interpolation and extrapolation from observed values of the mixing fractions at a fairly small number of points.

The group compared observed concentrations of the main groundwater constituents with concentrations obtained from the mixing fractions that they calculated. This was done to identify deviations from simple mixing. On the basis of this the group identified a set of reactions that were considered to explain the differences. The group also found that the concentrations of Cl^-, δ^2H and $\delta^{18}O$ did not match the observations. They ascribed this to stochastic scatter in the data.

For some of the water samples, the group also recalculated their chemical composition taking into account chemical reactions in the following way. First, mixing fractions for the four reference waters identified in the M3 analysis were calculated. This was done not as in the M3 analysis, but on the basis that Cl^-, Na^+ and $\delta^{18}O$ are conservative (i.e. non-reactive tracers). Then the corresponding concentrations of the other constituents were derived. Finally, chemical equilibrium calculations were carried out with PHREEQC for each sample. The results matched the observed concentrations of the various constituents much more closely than the concentrations inferred from the M3 mixing fractions.

4.4.2 Comments

Equation (4.4) in Liedtke and Klennert (2001) contains a number of mistakes as stated. Firstly the dispersion term should be divided by the retardation. Second, the equation is, presumably, obtained by subtracting *c* times the equation for conservation of mass of water from the equation for conservation of mass of tracer, so that the advection term is in the form $v \cdot \nabla c$ rather than $\nabla \cdot (vc)$, and to give the source term $q(c\text{-}c^*)/R$. However, this should mean that the time derivative term is in the form $n\frac{\partial c}{\partial t}$, rather than $\frac{\partial (nc)}{\partial t}$ as stated. Third, with the definition of the dispersion term implied by equation (4.4), the velocity appearing in equation (4.5) should not be the Darcy velocity or specific discharge but the transport velocity, (which is equal to v/n). It should also be noted that the definitions given following the expression for the retardation appear to suggest that the density appearing in the expression for the retardation is the fluid density, whereas it should be the rock density. It is probably also worth noting that the expression for the retardation implies a definition for the quantity K_d that differs slightly from the normal usage for this term.

The description of the way in which numerical dispersion was introduced in the modelling is not entirely clear. This is important, because dispersion is the only mixing process that occurs within the geosphere, and it appears from the comments in the report that numerical dispersion may be the dominant contribution to the overall dispersion. Therefore, the calculated results may be determined more by the model for numerical dispersion than the value of longitudinal dispersivity quoted (which is 2.5 m). This makes it difficult to make comparisons with the results obtained using different models.

It would be useful to explain (possibly with figures) how properties vary over those fractures that have heterogeneous properties (NE-2, NNW-4 and EW-3). It would also be helpful to provide more explanation of how the fracture width and permeability vary in the vicinity of the tunnel

The modelling provides additional insights in two areas. Firstly, the transport model has been run both with M3 mixing fractions and with Cl^- and $\delta^{18}O$. This allows a comparison of the outcome of indirect modelling of chloride and $\delta^{18}O$ via the transport of M3 mixing fractions with direct modelling of transport of the conservative species. Some significant differences are revealed, particularly where brine and glacial reference waters have substantial proportions and therefore control Cl and $\delta^{18}O$ respectively. Errors in the transport modelling of M3 mixing fractions proportions appear to be the source of discrepancy, although it is not entirely clear how the mixing fractions were determined from the concentrations of the conservative tracers (Cl^-, Na^+ and $\delta^{18}O$). In particular, there is some ambiguity in this, as acknowledged in the report, and it is not clear how this was addressed. This is potentially important because it appears that the approach of deriving the mixing fractions from the conservative tracers leads to better agreement with the measurements than the M3 approach.

The group indicate that, overall, there is also a significant source of error in the interpolation of M3 mixing fractions from the grid of known data points for initial groundwater compositions on to the specific flow paths (i.e. the HCDs). It is possible that this error is greater than that arising from transport of M3 fractions (see Section 5.3). Perhaps of more concern for the acceptability of using M3 reference waters in the transport model is the 'smoothing' effect of using M3 fractions that is apparent in the graphical comparison of the patterns of mixing predictions based on M3 fractions and those based on Cl, $\delta^{18}O$ and δ^2H with observed inflow compositions at control points. The BGR group suggests that this smoothing indicates a loss of information by using M3 fractions, in contrast to the claim that M3 adds information that is otherwise lost.

Secondly, other individual solutes have also been transported in the expectation that many or all of these would show non-conservative behaviour when comparing model predictions with observed concentrations. This is the case, as is evident also with concentrations of the same solutes interpreted from modelled M3 mixing fractions. The BGR approach using the geochemical model PHREEQC is a more rigorous approach than is possible with M3, and is similar to the way that PHREEQC has been used in the inverse modelling by the Posiva/VTT group (see Subsection 4.8). The results are reassuring in that, by including reactions, the mixing simulations more closely replicate the observed solute patterns, although caution is required because it is not clear exactly how Cl, Na and $\delta^{18}O$ were used to calculate mixing fractions.

The modelling work is rather more exhaustive in a geochemical sense than the modelling by other groups except for VTT. It shows that the geochemical changes can be modelled with a lot of effort. It also suggests that a similar degree of agreement for compositions at control points can be achieved using simply Cl and $\delta^{18}O$ as measures of mixing rather than M3 mixing fractions. Indeed, it would be a useful exercise to devise a way of objectively comparing the goodness of matches and a measure of the sensitivity of the two mixing models in terms of discriminating between transport model parameters and/or alternative geometries. Using $\delta^{18}O$ as a measure of fit emphasises the glacial water component, and Baltic water to a lesser degree. Using Cl as a measure of fit identifies the contrast between the brine, Baltic and meteoric water components. This may, in turn, 'tune' the transport model more for the parameters that affect these components, e.g. storage of matrix, connection of fractures towards the seabed, etc.

4.5 CRIEPI (Hasegawa et al., 2001)

4.5.1 Key Points

The groundwater flow and transport model developed by the CRIEPI group represented both the HCDs and the HRDs between them. A finite-element approach was used. The grid has a basic rectangular structure. The HCDs were not represented explicitly, but implicitly using a ‘smeared fracture model’ that integrates the properties of an HCD into finite elements that it crosses. These elements were assigned properties that were a volume-weighted average of the properties of the HRD and the HCD. The tunnel was represented using 1D elements on which the measured flows to the weirs were imposed.

Flow calculations were first carried out using parameter values based on Rhén et al. (1997b). A study of the sensitivity of the calculated heads at the measurement locations to the hydrogeological parameters was carried out. Using the results of this study as a starting point, the model was calibrated to try to match the measured heads up to December 1996. The effects of density variations were apparently taken into account in the groundwater flow calculations, using the Boussinesq approximation.

Although the FEGM-B groundwater flow model is said to deal with unsaturated seepage and non-linear boundary conditions such as occur at the tunnel face, it is not explained how these processes were included, if at all, in the model. The upper boundary condition seems to be a simple constant flux determined by modelling of the pre-tunnelling head distribution.

Then calculations of the transport of M3 mixing fractions (treated as conservative tracers) and the conservative tracers, Cl^- and $\delta^{18}O$ were carried out. In order to avoid numerical oscillations, an upwinding approach was used. The model was not calibrated using the measured concentrations, but the calculated values at the measurement locations were simply compared with the measured values. The calculated values generally differed significantly from the measured values. Then a backward pathline from a selected location was computed.

An attempt was also made to use the concentrations of helium (^4He) to increase understanding of the flow system. Steady-state calculations of the helium concentration were carried out for conditions before and after tunnel construction, and the calculated concentrations at the sample locations compared with measured values. The calculated concentrations were of the right order of magnitude, but a trend of increasing concentration with depth was not well reproduced.

Finally, the effects of various chemical reactions during mixing of reference waters to achieve the calculated groundwater mixtures were calculated. This was done using HARPHRQ (a variant of the PHREEQ model). Reactions modelled were: calcite dissolution/precipitation, organic C decomposition to produce HCO_3^-, oxidation of pyrite by O_2 and the HS/SO_4 redox equilibrium, and Ca-Na cation exchange.

4.5.2 Comments

The implicit approach adopted to represent the HCDs will give a reasonable approximation, but it will not generally be as accurate for a given level of discretisation as approaches in which the HCDs are modelled explicitly.

It should be noted that the upwinding approach adopted in the transport calculations will introduce numerical dispersion. In the outer parts of the model, where the elements are large, the numerical dispersion may be comparable to the physical dispersion that it is intended to model.

This report provides brief discussions of the reasons for changing the parameters in which the main changes away from the initial parameter values were made, identifying the observations for which the match is improved. These discussions provide the hydrogeological rationale for the varying relations between heads, inflows and progress of the tunnel. The diagrams of calculated versus measured drawdowns are too small to assess the match of model versus data, although it seems that there are very sharp transient excursions in the simulated drawdown versus time curves that require explanation (i.e. in KAS02, KAS04, KAS05, KAS12).

It is noted in this report that the water budget of recharge on Äspö Island versus total drainage into the tunnel almost certainly dictates that Baltic water will be drawn down towards the tunnel. However it is also acknowledged that the contribution of matrix storage is an unknown factor in this water balance, because the model here ignores the matrix.

A novel aspect of the group's work on Task 5 is the inclusion of a study of helium abundances in sampled waters and comparison of the measurements with values predicted with a helium *in situ* production and transport calculation. Helium could be a sensitive additional conservative tracer (along with Cl and $\delta^{18}O$) of flow and mixing, and more explanation and discussion of the He studies would be interesting, although this particular topic is probably outside the scope of Task 5. Radiogenic ^4He increases by about a factor of 10^3 between 70 m and 400 m depth in the undisturbed groundwater system prior to tunnelling. It could therefore be a very sensitive tool for distinguishing between water masses, either as an additional constituent in the M3 or chemical components approaches (see Subsection 4.7), or as an individual transported constituent. In water samples taken after tunnel construction, reported ^4He contents decreases by factors of between 10^1 and 10^4 relative to the corresponding undisturbed samples. Moreover ^4He data no longer show the pronounced increase with depth, indicating drawdown of younger water with less He. Therefore, ^4He changes might be a good way of resolving uncertainty about the extent of upconing of saline water from below the tunnel.

Results of geochemical reaction modelling of mixtures of M3 reference waters and of mixtures based on FEGM/FERM transport of conservative tracers (Cl and $\delta^{18}O$) are shown graphically and appear to be fairly similar though the details of the plotted results are not explained and the logarithmic scales for concentrations make the plots very insensitive. The conclusion drawn by the CRIEPI group is that the production of HCO_3^- is an important reaction that is not adequately simulated unless organic C decomposition is included in the reactions.

4.6 Enresa/UdC (Molinero et al., 2001)

4.6.1 Key Points

The stated primary objective of the Enresa/UdC group was ‘to validate (to the extent that is possible) current Thermo-Hydro-Geochemical codes for coupled water flow, heat transfer and multicomponent reactive transport. In other words, the objective is to test the ability of these codes to cope with the complex hydrogeological and hydrochemical settings which are expected to be found in a real HLW repository’.

In the numerical model, only the HCDs were represented. They were modelled using 2D finite elements, together with 1D finite elements to represent intersections between the HCDs and to represent the tunnel and shaft. The advance of the tunnel was represented using time-varying leakage coefficients for the nodes associated with the tunnel. The leakage coefficient for such a node was zero before the tunnel reached the node.

Several steady-state groundwater flow calculations, not taking account of density variations, were used to check the model and to begin the process of calibration. The transient groundwater flow model was then calibrated by manual adjustment of the model parameters to try to match the inflows to the tunnel and the measured drawdowns at the various control points up to 788 days after the start of tunnel construction. The initial values of the parameters were based on the values reported by Rhén et al. (1997b).

The group considered the match between the measurements and the corresponding values in the model to be generally good, although there were some discrepancies.

A transient calculation of the transport of the conservative species, Cl and $\delta^{18}O$, was then carried out. The initial distributions of Cl and $\delta^{18}O$ on the elements representing the HCDs were obtained by linear interpolation from the regular grid of values provided as part of the Task input (see Subsection 2.2). The parameter values were based on the values reported by Rhén et al. (1997b), and were not calibrated in this work. The resulting match to measurements of chloride in inflows and in borehole samples was considered to be generally good, with a few exceptions.

A suite of sensitivity studies was then carried out, in which aspects of the model were varied, and the change in the match to observations examined, including an alternative initial distribution for chloride, which was obtained by kriging from borehole observations and points representing the Baltic sea and Äspö island. It was concluded that the main uncertainty was that associated with the initial condition.

Transient calculations of flow and transport of chloride were carried out to times greater than the times of the measurements used in the calibration of the flow model. Calculated heads and concentrations of Cl were compared with observations. Generally the match was considered to be reasonable, although discrepancies were identified. Possible explanations for one discrepancy were suggested as heterogeneity within individual features, or the presence of an unidentified feature that is not represented in the model.

Finally transport calculations were carried out in which the M3 mixing fractions were treated as conservative species i.e. they obey the advection-dispersion equation. The initial distributions were obtained by interpolation from the grid of M3 mixing fractions supplied as part of the data delivery (see Subsection 2.2).

In addition to the main modelling task, Enresa/UdC used their CORE-2D model to simulate the evolution of groundwaters that have been sampled in the 'redox zone'. The redox zone is the first major fault zone intersected by the tunnel and was the subject of intensive monitoring in the early stages of HRL construction (Banwart et al., 1999). The CORE-2D computer code iteratively couples transport and geochemical reactions in a two-dimensional model and considers a large number of chemical components with acid-base, redox, and ion exchange reactions and mineral precipitation/dissolution. Two outcomes of this local model are of interest. Firstly it shows the sensitivity of groundwater compositions at this shallow location to disturbance by tunnel construction of the interface between fresh meteoric recharge and saline Baltic water. Secondly it couples the flow and mixing system with geochemical evolution, involving specifically the oxidation of both dissolved organic carbon and sulphide, to give an improved simulation of the reactions that were inferred by Banwart et al. (1999).

4.6.2 Comments

Without the qualification, the stated objective would be far too bold. In view of the believed dominance of mixing in the groundwater system at Äspö, and the uncertainties, it would not be realistic to expect that analysis of the data from Äspö would be able to provide much support for models of *reactive* transport.

The effects of the sensitivity variants were presented graphically using scatter plots of the difference between measurement and calculated value in one model versus the corresponding difference in another model. Such plots provide a powerful way of presenting a lot of information, but are quite hard to understand.

The group point out that calibration of their flow model with heads is reasonably good except that the modelled sharpness of changes is generally greater than is seen in measured head responses. This is attributed to diffusivity of the rock mass domain not being modelled in order to save computing time. They suggest that this might be compensated for by adjusting the storativity values for fractures. However it seems that, since the overall exercise is to calibrate a transport model, this may be losing information abut matrix storage. Although the group point out that the resulting flow model still gives 'very good' reproduction of inflows, this raises a question of how sensitive is the overall calibration exercise. The group did not recalibrate the model for transport, indicating that the resulting matches of simulations versus measured compositions were felt to be as good as could be achieved. As in the modelling carried out by BGR/BMWi (see Subsection 4.4), the transport model testing was done using both M3 fractions and Cl and δ^{18}O. The latter two gave 'very good agreement' at most control points.

In assessing the match of calculated chloride concentrations to observed concentrations at times later than those of the observations used to calibrate the flow model, the results of calculations are presented for two different initial conditions, and it is implied that the match is acceptable because the measurements lie between the results of the different calculations. However, this is not sufficient to justify a view that the match is acceptable. In several cases, the general trend of the observations differs significantly from the trend of the calculated values for either calculation. For the match to be acceptable, the initial condition should be within the range of possible initial conditions that would give an acceptable match to the observed trend. It is possible that this might be the case, but the presented information is not adequate to justify it. The forward predictions in many cases start at values that are known to differ substantially from the measured values. This of course is a poor basis for predictions and cannot possibly give an acceptable match. The predicted trend of changes may be a reasonable match, but the way that results have been calculated does not show this.

The group seems to conclude, probably correctly, that further efforts to 'fine tune' the transport model parameters and geometry would have little point because the overall calibration is dominated by dependence on initial conditions. They also point out that achieving a better match for M3 mixing fractions than for individual species, i.e. Cl and $\delta^{18}O$, would 'make no sense'. As the BGR group concluded (see Subsection 4.4), this raises the question of whether using M3 mixing fractions rather than the Cl and $\delta^{18}O$ to calibrate the transport model has any advantages, in view of the 'smoothing' effect of M3 mixing calculations and the sources of error in transporting M3 mixing fractions.

A final comment about the interpretation of their model results concerns the objectivity and consistency in evaluations of results. It is stated that 'a very good agreement' is found, in spite of the many caveats that are discussed. This optimistic evaluation is not really very objective, and the reader could equally conclude that the criteria for measuring success are not usefully rigorous or that the method itself is not very sensitive to parameters that are known to be uncertain or erroneous.

4.7 JNC/Golder (Dershowitz et al., 2000)

4.7.1 Key Points

The groundwater flow and transport model developed by the JNC/Golder group was based on work undertaken by this group within the Task Force on earlier tasks (whereas some of the other groups were unable to do this because they only participated in Task 5). The model developed by the group for Task 3 was used as the starting point for the work.

The models used were based on a Discrete Fracture-Network (DFN) approach. The HCDs were represented deterministically, and in most of the models considered, a realization of a network of random 'background' fractures was used to represent the HRDs between the HCDs. Earlier studies had identified step drawdown responses due to tunnel construction as one of the main reasons for difficulties in matching the calculated heads to observations, and it was suggested that these responses might be due to an unidentified feature. Analysis of the data suggested a possible location for the feature, which was included in the model. The tunnel was not represented explicitly in the models. Rather the flows into the tunnel were imposed. Once created, the DFN models were reduced to models of networks of pipes, in order to reduce the computational resources required for the calculations.

First the model was calibrated to try to match the observed heads (to December 1993). In this stage, various aspects of the model, such as the ‘skin’ associated with the Baltic seabed were modified, but the transmissivities of the HCDs were kept at the values in the model used for Task 3. The group emphasised the importance of including the background fractures.

Then transport calculations were undertaken for the M3 mixing fractions (which were treated as conservative tracers). The initial distributions were obtained by interpolation from the grid of values supplied as part of the data delivery (see Subsection 2.2). The transport calculations were carried out using an approach in which dominant pathways to the monitoring locations were determined from the calculated flows in the pipe network (using a graph-theory approach), and then the evolving concentrations at the monitoring locations determined from the transport of the tracers along these pathways.

The mixing fractions calculated from this model did not give a very good match to the observations (to December 1996). Therefore, a second stage of calibration was undertaken, in which the hydrogeological parameters of the HCDs were modified. In addition, in order to improve the match of the distribution of glacial water in the model to observations, one of the features in the model was extended to the north, where substantial amounts of glacial water are present.

The group also undertook the following additional pieces of work. An analysis was carried out in terms of so-called ‘chemical components’ rather than M3 mixing fractions. The first step in determining the chemical components is to carry out a principal components analysis. Then the compositions of a number of chemical components are determined such that all the groundwater samples are, to a good approximation, mixtures of the chemical components. The components need not correspond to physical groundwaters, and the number of chemical components required is not specified a priori. The approach was developed because it was considered to be more adaptable for groundwater systems where there is not such a clear-cut physical distinction between end-members as for the groundwaters at Äspö. The group carried out analyses for several different numbers of chemical components.

Further, the approach adopted for the transport calculations was improved. In the original approach, the relative proportions of water flowing along each path in the transport model were not known. In the revised approach, particles were tracked through the network of paths. At each intersection particles randomly moved into one of the possible paths in proportion to the flows along the paths. The fraction of the total number of particles moving along a path then approximates the proportion of water flowing along that path. The approach also allows for the pathways themselves changing as the flow field evolves.

An alternative initial condition was developed, based on the view that the groundwater chemistry at a point will be dominated by the groundwater chemistry of the nearest HCD rather than simply obtained by interpolation between measurements as in the values supplied as part of the Task input. A procedure was developed for determining chemistry in the HCDs from the data supplied (see Subsection 2.2).

Finally a further calibration of the model was undertaken. The results were considered to achieve a good fit of both heads and chemistry.

4.7.2 Comments

It is believed that only a single realization of the stochastic background fractures was used, but this is not entirely clear from the report. If so then the modelling results have not investigated the potential sensitivity of the transport model to the representation or properties of the HRDs.

The approach of reducing the fracture-network to a network of pipes is a reasonable approach that will reduce the computational resources required. Nevertheless, it is an approximation. The errors in the calculated flow will probably be quite small, and the errors in the transport calculation will probably correspond to errors in a 'dispersion' length that are of the order of the spacing between fracture intersections.

In the approach adopted for transport calculations, dispersion is modelled in a very different way to the way it is modelled in the approaches adopted by many of the other groups. In those approaches, dispersion is represented as a diffusion-like process proportional to the product of the velocity and a dispersion length. In the approach adopted by Golder, 'dispersion' results from travel through the multiple pathways in the pipe network. In some ways, this is perhaps a more physical model. However, it does mean that there are not convenient parameters (i.e. dispersion lengths) controlling the extent of spreading, or mixing, that can be adjusted to try to calibrate the model. It is also possible that the approach may underestimate the extent of dispersion in an individual HCD.

The description of the method for deriving the chemical components is not at all clear. Clearer explanations of the defining characteristics of the chemical components and the way that they are obtained need to be given.

Apparently, the method relies less on 'expert judgement' than M3. This could have positive or negative implications. A purely statistical approach to identifying components is likely to result in some components not corresponding to physical groundwaters. The major components are given credibility in terms of their correspondence with M3 reference waters. The minor components dominantly correspond to solutes that are needed to explain variations in groundwater chemistry due to reactions. These minor components are not therefore indicative of flow-mixing and are of secondary importance in Task 5.

The chemical components approach appears to have some advantages over the M3 approach. It uses as many components as are necessary to characterise essentially all of the variability in the compositions of the groundwater samples (seven components in the case of the groundwaters at Äspö). As such, it is likely that it will provide a better description of the groundwaters than the M3 approach which tends to use only the first two principal components, and so does not represent all of the variability. The M3 approach represents only 70% of the variability in the groundwaters at Äspö. More principal components could be used with the M3 approach, but the approach would lose much of its simplicity if this were done.

Also, the chemical components approach avoids the extra uncertainty that results from the use of the central point in the M3 polygon to resolve ambiguities in the mixing fractions, although there may be other sources of uncertainty. In the chemical components approach, it is not necessary for every groundwater sample to have contributions from all the chemical components, whereas in the M3 approach, every groundwater sample (other than those on the boundary of the M3 polygon) includes contributions from all the reference waters. There may also be equally significant uncertainties associated with the minor chemical components.

It is not clear that the chemical components approach offers any significant benefit over simply modelling the transport of the various groundwater constituents (i.e. major ions and isotopes).

4.8 Posiva/VTT (Luukonen and Kattilakoski, 2001)

4.8.1 Key Points

The Posiva/VTT group undertook three main studies in Task 5. They carried out an analysis of the sampled groundwater compositions using the geochemical inverse modelling approach outlined below. The PHREEQC geochemical model code was used for this (Parkhurst and Appelo, 1999). This takes into account both mixing and reactions, quantifying sequences of mixing and geochemical reactions that lead to the sampled waters from a number of suitable reference waters. These are identified on the basis of physical and chemical understanding of the evolution of the groundwater system.

The fractions of each reference water that go to make up a particular water sample were determined as follows by the group. A sequence of feasible simple mixing and reaction steps are identified that start from reference waters and ultimately lead to a water with the composition of the sample, to within the uncertainties in the analysis of the composition of the samples. At each step, two or three groundwaters are taken to mix. The fractions of each of the mixing groundwaters in the mixture are determined from the concentrations of Cl and $\delta^{18}O$ in the sample under consideration and in the mixing groundwaters (Cl and $\delta^{18}O$ are usually considered to be conservative, i.e. non-reacting and non-sorbing, tracers). The concentrations of the other groundwater constituents in the resulting water are determined by modelling reactions that are considered to be occurring, such as dissolution and precipitation of calcite, consumption of organic matter, precipitation of pyrite and ion exchange processes. The groundwaters that are taken to mix in each step are determined by a trial and error process supported by understanding of the nature of the groundwater system. Once a sequence of feasible mixing and reaction steps has been identified, the overall fractions of each reference water that combine to give the sample are determined by following the analysis from the reference waters to the sample.

This led to an alternative interpretation to that provided by the M3 analysis. In the new interpretation, the groundwaters at Äspö were interpreted as the result of mixing of seven reference waters (and reactions between these waters and the rocks) rather than as the result of the mixing of four reference waters as in the M3 analysis. The analysis also led to an alternative initial distribution for chloride.

The VTT group also developed two models for groundwater flow and transport. The first of these models addressed transport of the M3 mixing fractions. It represents both the HCDs and the HRDs in a finite-element model. The HCDs were represented using 2D elements, and the HRDs were represented using 3D elements. In the model, the effects on the flow of the variation in groundwater density resulting from variations in salinity were taken into account.

The tunnel was represented by means of an appropriate imposed head (strictly, residual pressure) imposed on the nodes corresponding to the tunnel. It appears that the measured flow rates were only used to impose the boundary conditions for the transport calculations.

The model was calibrated to match the measured freshwater heads and the flows to the tunnel. Data up to May 1993 were used. Transport calculations up to December 1996 were then carried out. The model was calibrated to try to improve the match to the observations, by adjusting, for example, the transmissivities of some of the HCDS. The final match achieved was generally acceptable, although there were some discrepancies, particularly for KR0012B. It was suggested that the large discrepancies observed for KR0012B were due to the large size of the elements locally.

Backward pathlines were calculated to indicate the origin of the water reaching particular sample points.

A similar model was also developed and used in a similar way to carry out calculations of the transport of the mixing ratios of the seven reference waters obtained from the geochemical inverse modelling approach.

4.8.2 Comments

We believe that the model is as described above, but the report is not entirely clear in its description of the model. In particular, the mathematical formation presented is that for a dual-porosity model, and there is perhaps an implication that the HRDs are modelled as the matrix blocks between the water-bearing fractures, although it is believed that the dual porosity formulation may not have been used. In the finite-element representation adopted, what level of discretisation is adopted?

There may be an apparent inconsistency in the treatment of the inflows. It appears, as noted above, that the measured inflows were not used to calibrate the modelled inflows of solutes to the tunnel. However, the inflows to the tunnel in the model would differ from the measured inflows, because the former are determined by the imposed head on the tunnel. There would therefore be an implied inconsistency. It is possible that the view is taken that the flows in the model do not correspond to the real inflows which will be strongly influenced by the grouting that has taken place in the vicinity of the tunnel, which is not represented in the model, and therefore the approach taken is the most realistic for the chosen model. However, if so this really needs to be explained and justified.

In general, the details of the calibration procedure for both the flow and the transport models are not explained clearly. For example, was only the salinity distribution used to calibrate the transport model, and was calibration aimed at matching measurements at all times? If so, the large discrepancies in KR0012B are not adequately explained.

It would have been useful to give the travel times along the backward pathlines.

The time discretisation in the model is quite crude (only 17 time steps were taken). This could lead to numerical errors. It is recognised that it may not have been practicable to adopt a significantly finer time discretisation.

There are important differences between the inverse modelling approach to using geochemical information and the M3 approach. In the geochemical inverse modelling approach, the mixing fractions are determined in a more realistic and physically based way than in the M3 approach. In the geochemical inverse modelling approach, effectively, the potential ambiguity in determining the mixing fractions for several reference waters from just two variables (the concentrations of the conservative tracers Cl and $\delta^{18}O$) is resolved by the requirement that the concentrations of the other groundwater constituents should be the result of feasible geochemical reactions (which are quantitatively modelled), whereas in the M3 approach this ambiguity is resolved by a mathematical artefact (the introduction of the central point with specified mixing fractions).

In the geochemical inverse modelling approach, the reference waters are not restricted, but may be any set of waters that have physical significance, taking into account the palaeohydrogeology and palaeogeochemistry of the site under consideration; whereas in the M3 approach the points corresponding to the reference waters must be the nodes of a polygon in the M3 plot containing the points corresponding to all the samples. In particular, for M3 as currently implemented, it is not possible to use as a reference water a water corresponding to a point in the interior of the polygon, even though such a water may be of considerable physical significance at a given site.

The method may be difficult to use conclusively, or have high conceptual uncertainties, in systems that are less well defined by conservative parameters than is the Äspö system, that is in systems where reactions are more important. The same difficulty would anyway apply to both the M3 and chemical components approaches, which are based on an assumption that mixing is the dominant process.

The geochemical inverse modelling approach is more complicated and is certainly more laborious than the M3 approach. It is more credible from a geochemical point of view because the interpretation is explicitly consistent with evolution by mixing and reactions, although in another way it is less transparent because there is a large element of expert judgement in selecting end-members, ‘flow/mixing pathlines’, and the identification of the sequence of reaction steps leading to each groundwater sample.

4.9 SKB/CFE (Svensson et al., 2002)

4.9.1 Key Points

The SKB/CFE group (which included GeoPoint and Duke Engineering) carried out the M3 analysis of the geochemical data that formed the basis of the data delivery of groundwater compositions. This analysis led to the identification of four reference waters (Meteoric, Baltic, Glacial and Brine), and to mixing fractions for each groundwater sample, that is the fractions of the sample that correspond to the reference waters. The calculated mixing fractions were supplied to the groups participating in Task 5. The mixing fractions were also interpolated/extrapolated from the sample locations to the nodes of a rectangular grid (using the Voxel Analyst program) and this information was made available to all the participating groups (see Subsection 2.2).

The group carried out a simple test of the validity of the assumption that the groundwater compositions were determined by mixing of the reference waters. This is to some extent a test of the internal consistency of the M3 approach for the Äspö groundwaters. For each groundwater sample, the composition that would result from mixing of the reference waters with the calculated mixing fractions was evaluated and compared with the actual composition. It was found that there was reasonable agreement for the conservative tracers, but there were significant deviations for the reactive tracers. These deviations were interpreted as the result of water-rock interactions.

A study of the changes in groundwater composition that result from tunnel construction found that they were not simply related to depth or hydraulic conductivity.

The group also undertook the following analysis, which attempts to predict the changes in groundwater compositions with time in the vicinity of the tunnel. The sample locations were classified into groups on the basis of the dominant mixing fraction in the sample. Then for each group the average rates of change in the different mixing fractions due to tunnel construction were calculated. These average rates of change were used as the basis for forward projection to determine estimated changes, which were then compared with actual observed changes.

The group carried out various studies to examine issues related to the use of the M3 approach. In order to assess where the procedure for resolving the ambiguity in the M3 mixing fractions leads to excessively large errors in mixing fractions for particular reference waters, they examined the correlation between the mixing fraction for glacial water and $\delta^{18}O$ (which is a sign of water with a cold-climate origin). They found a good correlation. They also examined the inverse correlation between the mixing fraction for meteoric water and chloride concentration [Cl], which they considered to be good.

One aspect of the M3 approach is that the mixing fractions for a groundwater sample do not depend only on the compositions of the sample and the reference waters, but on the compositions of all the samples used in the analysis. In order to examine the implications of this, the group compared the mixing fractions obtained from an M3 analysis based on the limited data available before tunnel construction with those obtained from the full data set. They found that the changes were fairly small and were less than the uncertainty associated with the M3 mixing fractions.

The group developed a model for groundwater flow that represented implicitly both the main features (the HCDs) and the fractured rock mass between these. The numerical approach was basically a finite-difference method in which the hydraulic conductivity of each grid block in the model was chosen to represent both the HCDs crossing the block and the fractures in the rock mass within the block. The fractures were modelled stochastically.

The initial flow and transport model did not include the stochastic fracture network representing the rock mass. This model corresponded to a site-scale model developed in previous work by the group. The pressure boundary conditions for this model were obtained from a regional-scale model (10x10x3 km). This model was regarded as adequately calibrated from the hydrogeological point of view. It was found that the initial assumption about the salinity distribution on the boundary of the model led to an adequate match to the measurements of groundwater composition before tunnel construction and when the tunnel front was at 3170 m, so the model was considered to be acceptable without changes.

The unsaturated zone near the ground surface was taken into account using an approximate method, in which, rather than modelling the unsaturated flow equations, the horizontal hydraulic conductivity was reduced to a level at which the horizontal flow was negligible for grid blocks above the water table (where the pressure is zero).

After the fracture network in the rock mass was taken into account, the model was calibrated. This was done in three stages. First the hydraulic conductivity of the near surface region and the transmissivities of the HCDs were adjusted to give a match to the initial water table and the pressure responses in the boreholes. Then the kinetic porosities were scaled to give a match to the changes in salinity resulting from the tunnel construction. Finally the assumed water salinity on the boundary was adjusted to try to match: (i) the initial water composition, (ii) the composition when the tunnel was at 3170 m and (iii) the composition in May 1996. Five realisations of the stochastic fracture network in the rock mass were considered and the one that gave the best match to observations was taken as the calibrated model.

The group carried out various calculations to assist in understanding the behaviour of the model, including calculations of backwards pathlines to various control point so that the source of the water reaching these points could be identified. It was found that the travel times to the control points from the boundary of the domain were very short, and at later stages most of the water entering the tunnel is modelled to originate from the domain boundaries. This raised the question of how water compositions outside the modelled domain might be affecting the compositions of inflows. A related problem is how to account for the apparent preservation of large fractions of glacial water at a few hundred metres depth below Äspö (see below). This appears to need larger storage volumes than are represented by the major HCDs alone. It is suggested that connectivity and storage volumes need to be re-examined to improve the reliability of continuum models for transport.

In order to explore the sensitivity of the results to the parameters, the group compared the calculated groundwater compositions with those obtained from different realisations of the fracture network. The compositions were found to vary significantly between realisations.

The modelling identified the following issue. Calculated groundwater travel times in the model are quite short. The time to travel from the boundary of the domain to the vicinity of the tunnel is of order a year. The fact that the travel times are quite as short as this is a consequence of the high head gradients due to the presence of the tunnel, but nevertheless, this raises the issue of how the glacial component of the groundwater has remained since the last ice age more than ten thousand years ago. A possible mechanism by which this could occur was identified. If the zones at which groundwater enters and leaves a nearly vertical fracture are well above the bottom of the fracture, and the groundwater near the bottom of the fracture is denser than the water flowing through the fracture, the denser groundwater will tend to remain in the fracture. Similarly, water that is lighter than the water flowing through the fracture can be trapped at the top of the fracture. Calculations for a simple model demonstrated this effect.

4.9.2 Comments

We do not believe that the attempt to predict the groundwater compositions on the basis of the average rates of change of the mixing fractions is very useful. Essentially this is a (weak) test of the linearity of the change in mixing fractions with time. However, it would be expected that the change in composition at a given point would be highly non-linear as a function of time. (In general, the composition might reflect the movement of one or more mixing zones past the point.) Further the changes predicted are generally much smaller than the uncertainties associated with M3 mixing fractions, so it is not clear that any significance can be attached to the comparisons. Also, the test cannot really be described as predictive, because all the data were used to derive the rates of change of the mixing fractions.

The appendices in the SKB/CFE report provide several valuable sensitivity investigations that shed light on the pros and cons of using M3 as the tool for representing hydrochemical information in Task 5. These indicate that:

- M3 mixing proportions are fairly sensitive to the selection of reference waters – for example, omitting the ‘modified sea water’ reference water adds errors up to about ±0.1 in calculated fractions for some samples;

- Typical analytical uncertainties have a relatively insignificant effect on calculated mixing fractions;

- The M3 modelled fractions have more significant degrees of non-uniqueness, and thus potential error above the ±0.1 indicated, when the composition plots near to the centre of the M3 polygon;

- Using only the first two principal components (PCs) in the M3 model has lost about 10% of the information about variance compared with using the first three PCs. However most of this additional information pertains to tritium which was subsequently excluded from the data set anyway;

- Carrying out the PCA with conservative species only, i.e. Cl, $\delta^{18}O$ and $\delta^{2}H$, produces an M3 plot in which, as expected, the data points and the inferred reference waters are slightly more compact in PC-space. However, it is not entirely clear that, as claimed by the SKB group, the overall uncertainties are reduced by the use of the non-conservative species as well as the conservative ones. Using all the species may make it slightly easier to identify the reference waters. However, the use of the non-conservative species introduces additional uncertainties. This view seems to be supported by the change to the shape of the M3 plot obtained by reconstructing the sample data using the estimated M3 fractions and assuming that all species are non-reactive. The overall impression is that the M3 plot and consequent mixing calculations have a degree of uncertainty, possibly more than the ±0.1 suggested, that is difficult to pin down.

A significant finding from this study has been the uncertainty and potential error in the parameterisation of the transport model, especially with respect to matrix storage and kinematic porosity, that is revealed by the M3 mixing fraction tests. In particular, the glacial water fraction, which is conceptualised as a finite reservoir of palaeorecharge water, is found to be a rather sensitive test. It may be that the same outcome could have been achieved by an analysis using $\delta^{18}O$ and Cl rather than M3 fractions. Another view of this finding is suggested by the modelling by the JNC/Golder group (see Subsection 4.7), who choose to change the geometry of conductive fractures and the boundary conditions rather than changing the storage of a finite rock mass domain. This illustrates how the approach in Task 5, of modelling being developed by many groups, has revealed alternative concepts and expanded uncertainties in the flow/transport model that might otherwise not have been apparent.

The benefit of M3 as a tool for visualising compositional variations, and for identifying probable end-members, in a mixing-dominated groundwater system is apparent in the M3 plot. This is particularly well illustrated for the Äspö HRL data set. The SKB group's report provides some illustrations of how this visualisation can be taken a step further to produce a simple illustration of how particle tracking flow lines output by the flow model can be tested for consistency with expected spatial distribution of different water masses. For example, flow lines from depth have higher proportions of brine, flow lines with angled trajectories tend to correspond to more Baltic-type water, etc.

Final comments concern uses of M3 to (a) predict forward trends of inflowing water compositions from time-varying patterns of M3 fractions in past inflows, and (b) infer geochemical reactions that are the causes of various solutes having non-conservative behaviour. In the first case, averaging of graphical patterns of calculated M3 fractions has been used to extrapolate rates of compositional change. It can be seen that this approach makes many assumptions and simplifications, for example that the trend of change overtime remains uniform, which in turn assumes that initial compositions vary uniformly along the flow paths. The validity of this approach can be assessed by comparison of a 'prediction' of inflow compositions beyond a series of observed inflow compositions that are used as a calibration data set.

In the second case, deviations of individual data points for reactive species from a conservative mixing trend have been interpreted to indicate the extent of reaction. A general comment on both cases is that outputs from M3 are being used to interpret and potentially to quantify processes when the uncertainties in both the processes and in the validity of using M3 fractions quantitatively are poorly constrained. In simple terms, it is difficult to conceive an application of these rather uncertain results that would be sufficiently reliable for predictive and interpretative purposes. Forward predictions of groundwater composition changes will be closest to being 'fit for purpose' (whatever that purpose might be) only if an adequately-calibrated flow-transport model is used. Interpretations of geochemical reactions and mass transfers are more reliably and transparently carried out by using fully quantitative and calibrated mixing and reaction models such as PHREEQC with discrete water samples.

The extent to which the suggested mechanism for preserving glacial water in the system would be effective for a realistic fracture network is unclear.

5. Models and Approaches

In this Section and the next, the work that has been carried out on Task 5 is reviewed. The work must be viewed in context. Task 5 was not a repository performance assessment. Therefore, it should not be expected that the modelling or its reporting would be as detailed as that appropriate to an actual performance assessment. Further, the work that could be carried out by the participating groups depended on the resources available to them, and in some cases was constrained because the groups only participated in Task 5 at a late stage. This should be taken into account in considering the discussion of the work of the groups. Nevertheless, it is important to bear in mind that that an actual repository performance assessment would probably require more detailed modelling, and it would need to be justified in more detail than the modelling in Task 5.

In this Section, the models and approaches used for Task 5 are reviewed. In Subsection 5.1, the conceptual and numerical models used by the participating groups are discussed, and in Subsection 5.2, issues relating to the initial conditions are considered. In Subsection 5.3, issues relating to the use of the M3 approach are addressed, in Subsection 5.4, the approaches adopted to model calibration are reviewed, and in Subsection 5.5 uncertainties are discussed. In Subsection 5.6, some comments on the presentation in the final reports of the groups are made. Finally, in the next Section, the progress that has been made in the integration of geochemistry and hydrogeology as a result of Task 5 is reviewed.

5.1 Models

The groundwater flow and transport models developed by the groups were all based on the same underlying conceptual model. This model, which is described in Rhén et al. (1997b), is based on the very extensive site investigations carried out at Äspö and is the result of work outside Task 5. In the conceptual model, groundwater flow is predominantly through the Hydraulic Conductor Domains (HCDs), with weaker flows through the Hydraulic Rock-mass Domains (HRDs) between the HCDs. Although the modelling groups were free to modify the geometry of the HCDs, they all based their models on the geometry of the model of Rhén et al. (1997c). This geometry could be considered to be reasonably well established. In both the HRDs and the HCDs groundwater flow is through fractures, rather than the rock-matrix between the fractures. However, the solutes travelling with the flow could diffuse between the fractures and immobile groundwater in the matrix. It is perhaps worth noting that the terminology adopted by the groups might be confusing to those unfamiliar with the Task. Many groups referred to the HCDs as fractures, although an HCD is not an open void with aperture equal to the thickness of the HCD, and some groups appeared to refer to the HRDs as ‘the matrix’, although as indicated above, the groundwater flow through the HRDs is predominantly through fractures.

However, there were considerable differences in the simplifications that the various groups made to this model and in the numerical representations that they adopted. Most groups modelled similar regions with dimensions 2x2x1 km (which is similar in size to the original site-scale model developed by SKB, 1.8x1.8x1 km), although some groups modelled slightly different regions. Partly as a result of this, the models of the different groups represented different combinations of HCDs. Further, JNC/Golder found it useful to include an additional, unidentified feature in their model (see Subsection 4.7), and ANDRA/ITASCA included additional lateral connections between HCDs in their model. Some groups did not include representations of the HRDs in their models, because of the view that the flows in the HRDs are weaker than the flows in the HCDs, and to reduce the computational resources required. Most of the calculations appear to have been close to the limits of what was practicable for the groups. However, ANDRA/ANTEA, CRIEPI, JNC/Golder, Posiva/VTT and SKB/CFE did include some representation of the HRDs in their models.

For the underlying conceptual model, the neglect of the HRDs would not have an effect on the overall groundwater flow, although flows might be affected in small regions in the vicinity of less transmissive HCDS, where the HRDs might effectively provide flow paths with comparable transmissivity to the HCDs. The work of ANDRA/ANTEA (see Subsection 4.9), who compared the results of calculations with and without explicit representations of the HRDs, supports this view. However, the HRDs have a more significant effect on solute transport, as shown by the work of JNC/Golder (see Subsection 4.7). The HRDs may provide reservoirs for migrating solute. In those models in which the HRDs are not represented, their effect may have been taken into account to some extent through the use of enhanced storage parameters for the HCDs. The matrix between the fractures in the HRDs and the HCDs could also have a significant effect on transport, although the matrix was not explicitly taken into account by the groups.

It appears that in all of the models, the HCDs were treated as simple features (fractures) with a certain thickness. However, in reality, the HCDs would have internal structure. There is presumably considerable spatial variability in the properties of an individual HCD or HRD. The structure and variability were not taken into account by most groups. BMWi/BGR allowed for variability within some of the HCDs although probably on too large a length scale, and Posiva/VTT allowed for the transmissivity of the HCDS varying with depth, as suggested by the transmissivity measurements (Rhén et al. 1997). The internal structure of the HCDs may have effectively been taken into account to some extent through the parameters used to characterise the features (e.g. storativity, dispersion).

The available data show that there are significant variations in groundwater salinity and thus in groundwater density within the region under consideration. These variations would be large enough to significantly affect groundwater and transport within the region, and this is shown by the studies of, for example, ANDRA/CEA (see Subsection 4.2). However, in the models used by some of the groups the groundwater was taken to have constant salinity.

As the process of tunnel construction proceeded, the water table was lowered considerably (by up to about 80 m) in the region above the tunnel under Äspö island. As a result, the near-surface region became unsaturated, and should ideally be modelled as such. In practice, most of the models treated the flow as fully saturated up to the ground surface and used an imposed recharge boundary condition on the upper surface. The models will therefore be giving a reasonable approximation to vertical flows in this region, but may not be representing horizontal flows in this region very well. A related bias is that when the water table is lowered as a result of tunnel construction, the recharge will be significantly increased because the amount of run-off and evapotranspiration would be reduced. This was effectively taken into account by some, but not all, of the groups.

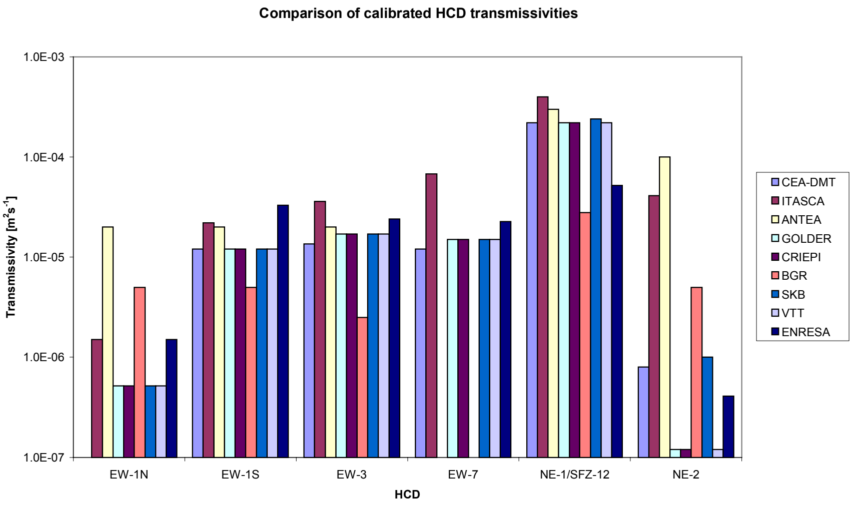
Flow and transport in the region considered by most of the modelling groups is significantly affected by the conditions on the lateral boundaries of this region. These conditions may have changed significantly due to the tunnel, and modelling by SKB/CFE indicates that they were (see Subsection 4.9), but this was not taken into account in any of the modelling. In all cases, the lateral boundary conditions were taken to be constant over time.

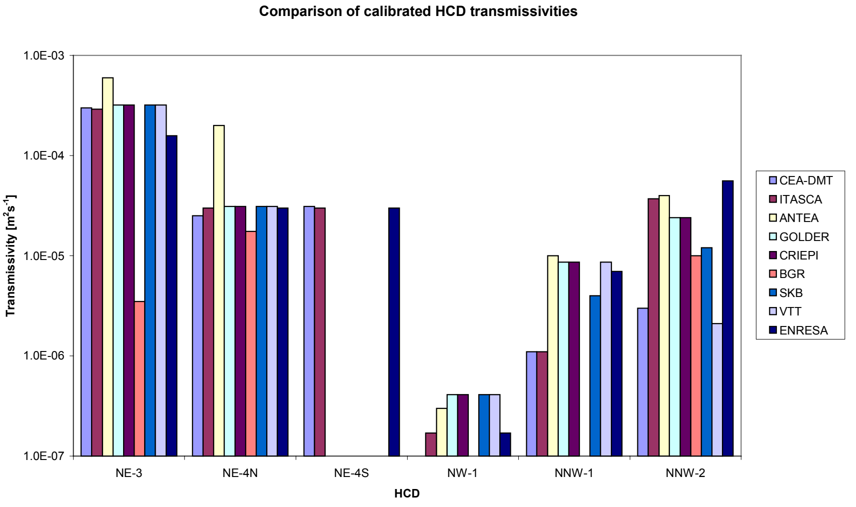
The numerical representations adopted by the various groups for the underlying conceptual model encompassed all the main categories of numerical models for groundwater flow: continuum porous medium models, discrete fracture-network models and pipe-network models. Many of the models had aspects of more than one category. For example, the model developed by Golder/JNC (see Subsection 4.7) was fundamentally a discrete fracture-network model, although this was further simplified to a pipe-network model for purposes of calculation. The approach that was perhaps most widely adopted by the participating groups was to represent the HCDs in terms of a three-dimensional network of features modelled effectively as two-dimensional porous media.

We consider that all of the adopted approaches to modelling provide reasonable approximations to groundwater flow and solute transport through the rocks at Äspö, given the underlying conceptual model. It would be expected that there would be biases in all the models as a result of the various simplifications discussed above, such as neglect of the HRDs, neglect of the effect of salinity variations, neglect of the transient variations in the top boundary conditions, etc. However, it would be expected that those models in which fewer approximations of the underlying conceptual model are made might be better, or more realistic.

The levels of discretisation adopted in the various models, which are similar, appear on general grounds to be reasonable, although the only way to really assess this would be to carry out detailed studies of the effects of grid refinement. However these would, almost certainly, not be practicable given that the models may have been near the limit of what was possible with available computing resources. The magnitude of the change found by ANDRA/ANTEA (see Subsection 4.1) on switching from one finite-element formulation to another with the same grid is large. It suggests that results for both formulations may not be entirely grid converged.

We suspect that numerical dispersion may have been a significant, or even dominant, contribution to the overall dispersion in some models. Support for this view is given by the fact that, for the solute transport calculations, some groups found it necessary to adopt upwinding techniques, or approaches with similar effect. This is particularly significant because the interpretation of the geochemical information is based on the view that the groundwater composition is largely controlled by mixing, and dispersion is the only mixing process that is operating within the rocks when represented as a porous medium. (In the pipe-flow model, mixing occurs at the junctions of pipes.).





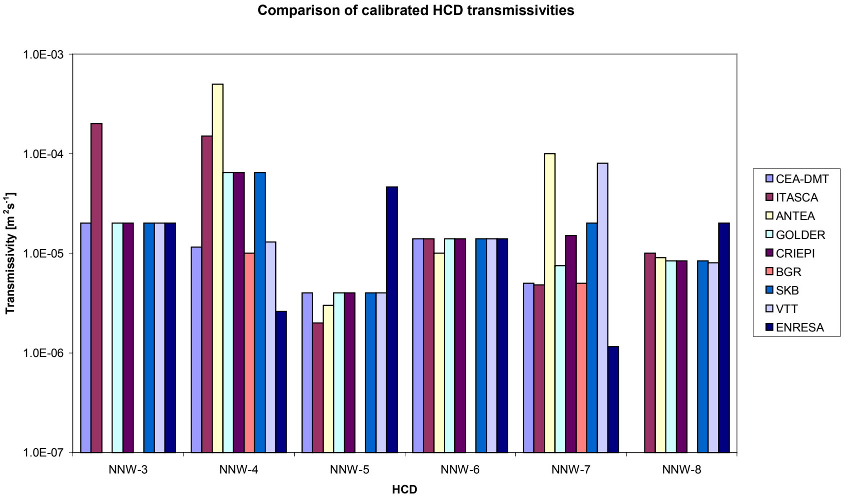


Figure 1-4. *Comparison of calibrated HCD transmissivities.*

One aspect of the results obtained by the various groups that is potentially of considerable interest is that, although they started from the same underlying conceptual model, and indeed the same recommended parameter values for the features in the models, the final models that they obtained were very different. For example, in some cases, the final calibrated transmissivities for the same feature differed by as much as three orders of magnitude (see Figure 1-4). This might reflect the existence of significant differences between the models. However, the differences might simply be the result of the different subjective choices made by the groups whilst calibrating their models, which could be essentially the same. This would probably mean that the calibrated quantities in the models correspond to observations are not very sensitive to the particular parameters adjusted in the calibration. In the latter case, the spread of the results obtained by the groups might give some indication of the range of parameter values that are consistent with the available data.

It is unfortunate, but understandable within the resource constraints, that none of the modelling groups has carried out a comprehensive assessment of the allowable ranges for all parameters. A systematic investigation of acceptable parameter ranges would probably be necessary in a future application of this approach within a repository performance assessment. It is perhaps worth noting that in models in which an HCD is represented by a feature with a uniform (effective) transmissivity, this transmissivity may differ significantly from the results of individual measurements within the feature. A measurement gives a measure of the behaviour of a local region within the feature, which may be very small if the measured value is low.

5.2 Initial Conditions

Many of the groups stressed the importance of the initial geochemical conditions in determining the results of the models. The initial conditions that underpinned most of the modelling were obtained by interpolating and extrapolating the measured groundwater chemistries for a fairly sparse set of observations to a rectangular grid. The interpolation was carried out using the program Voxel Analyst, which uses an approach based on kriging. Most of the observations were concentrated in the vicinity of Äspö island, with very few measurements further away. There may therefore be significant uncertainties about the initial compositions of groundwaters away from the vicinity of the measurements. This could be a serious source of uncertainty, especially in areas of very sparse measurements such as out at the model boundaries. This would be particularly important, if, as the model suggests, transport from these boundaries is fairly rapid.

To some extent, therefore, the predictions of the models were controlled by the extrapolation of the initial measurements rather than by direct measurements. This means that the match of the model predictions to observations provides less support for the model (i.e. the benefits of using the geochemical information are less) than would be the case were the initial conditions defined better by direct measurements. However, a match between predictions and observations does demonstrate that the model, with the assumed extrapolation of the initial conditions, is self-consistent. Nevertheless, more measurements, particularly at some distance from Äspö island, might have been useful and could have meant that the geochemical information provided more constraint on the flow and transport model. It might also have been useful to have explored the implications of alternative initial conditions (consistent with the observations), although it is recognised that what could be done within the framework of Task 5 was limited by the resources available for the work.

As indicated above, the initial conditions used in most of the modelling were obtained by a simple geometrical interpolation and extrapolation. In reality, the geochemistry of the groundwater would not vary smoothly between the measurement locations, but there might be fluctuations and step changes in the geochemistry. The Golder/JNC group also examined the implications of using an interpolation scheme that took more account of the physics of the flow (see Subsection 4.7). They found that this was beneficial. However, once the initial condition is determined in a way that takes the flow into account, the independence of the model and the measurements used to test it may become an issue.

5.3 M3 Issues

Much of the work undertaken on Task 5 used mixing fractions obtained from the M3 approach (see Laaksoharju et al., 1999a and Section 3). We therefore think that it is important that issues relating to the approach are briefly discussed here.

We consider that M3 approach provides a good way of presenting the geochemical information in terms that are probably readily understandable by those without geochemical expertise. This is because the approach gives a simple description in terms of mixtures of different reference waters. The M3 approach involves an objective analysis of data, although expert judgment is involved in the choice of the reference waters. At Äspö, understanding of the palaeohydrogeology aided this choice. The chemical components approach (see Subsection 4.7) also involves an objective analysis of data, but the geochemical inverse modelling approach (see Subsection 4.8) involves considerable expert judgment including interpretation of flow, although it is more realistic and physically based than either the M3 approach or the chemical components approach.

M3, geochemical inverse modelling and the chemical components approach are all less straightforward than describing the composition as a mixture in terms of the non-reactive (‘conservative’) concentrations of the constituents (such as chloride, bromide and $\delta^{18}O$) that are measured in groundwater samples. This approach is widely used and we believe that it is the approach that geochemists would be most comfortable with although it may not be as immediately appealing to non-geochemists.

M3 introduces additional uncertainties into the geochemical description as a result of the prescription adopted to remove the ambiguity if there are more than three reference waters (see Section 3). At 90% confidence level, the uncertainty is ±0.1, but significantly larger values (of order 0.5) are possible (see Part 2). As a result, the test of a model for transport of M3 mixing fractions on the basis of a comparison of the modelled mixing fractions with mixing fractions determined from of groundwater analyses is likely to be less stringent than a test of a corresponding model for the transport of groundwater constituents in which the concentrations of the constituents are compared directly with the measured concentrations. This means that the uncertainties associated with the model for the transport of M3 mixing fractions will be larger and the confidence in the model less.

In the M3 approach as applied to the data set for Task 5, reacting constituents were treated on exactly the same footing as the non-reactive constituents. An explicit assumption in M3 is that the groundwater compositions are determined predominantly by mixing of a number of chemically distinct water types or 'reference waters'. The use of the reactive constituents in the principal components analysis may help to distinguish the reference waters. Expert judgment is also necessary to identify the reference waters with meaningful water types. Thus the reacting constituents also influence the analysis to determine the mixing fractions for a water sample, an analysis in which all constituents are treated as mixing without reacting. This would appear to introduce an inconsistency, noting that the reactive nature of some constituents is then recognised in the final step of the M3 analysis, which aims to identify the main reactions. However, the philosophy of the M3 approach seems to be that it is an approximation, and the errors in the mixing fractions resulting from inclusion of reacting constituents are contained within the overall uncertainty associated with the approach. Nevertheless, we think that many geochemists would consider the use of the reacting constituents to be contentious and that a rigorous geochemical analysis would be preferable.

The outcome of the prescription for removing the ambiguity if there are more than three reference waters (i.e. the calculation of the mixing fractions via the introduction of the centre point in the M3 polygon) is that the mixing fractions do not actually obey the standard advection-dispersion equation, even if it is assumed that only mixing occurs, but not reactions. This is because the prescription makes the relationship between the M3 mixing fractions and the concentrations of the groundwater constituents non-linear (strictly piece-wise linear) rather than linear (see more detailed discussion in Part 2). As a result, the transport equation for the mixing fractions includes an additional term that is not present in the standard advection-dispersion equation. However, this was not taken into account in the work carried out for Task 5. The groups that modelled transport of M3 mixing fractions simply assumed that they obeyed the standard advection-dispersion equation.

One of the authors of this review has carried out a study (see Part 2) to examine the size of the error resulting from assuming that the mixing fractions obey the standard advection-dispersion equation. It was found that on average the error was very small, although in particular cases, the error could be very large (of order 0.5 in a mixing fraction in one case for example). It was also found that in a substantial fraction of cases, the initial direction in which mixing fractions change when two groundwaters mix would be incorrectly predicted. On average, the M3 approach probably gives an approximation that is acceptable in the context of uncertainties in other parts of the hydrochemical interpretation and modelling and of the transport model. However the significance of this approximation should be estimated and explained.

It may be noted that the computational cost of transport calculations with the M3 mixing fractions is also likely to be significantly greater than the computational cost of transport calculations for chloride and $\delta^{18}O$.

In the light of the comments above, we consider that the use of the M3 mixing fractions in the transport calculations carried out for Task 5 had no real technical advantages and had significant disadvantages. However, the rôle of the M3 approach in interpreting and visualising the hydrochemical evidence for groundwater mixing, which stimulated and facilitated the work of the Task 5 groups, is acknowledged.

5.4 Modelling Procedure and Calibration

The procedure that the SKB modelling group originally proposed to adopt in Task 5 is shown in Figure 1-1, and is discussed in Subsection 2.2. In essence, the approach that was suggested was as follows. A groundwater flow and transport model would be set up using a given structural model and hydrogeological parameters. Starting from conditions determined from observations before tunnel construction, the initial and boundary geochemical conditions would then be calibrated to match to the observations after tunnel construction. In this approach, it was not envisaged that the structural model and hydrogeological parameters would be changed. These were regarded as pre-defined, as a result of previous work at Äspö.

None of the participating groups used this scheme. In general, the groups first set up a flow model based on the conceptual model described in Rhén et al. (1997b). This model was calibrated to match the observed heads and flows by adjusting the hydrogeological (or flow) parameters. First, conditions prior to tunnel construction were matched and then the heads and inflows resulting from tunnel construction were matched. Then a transport model based on the flow model was set up, and calibrated to match the geochemical measurements of groundwater composition, by adjusting transport parameters such as dispersion lengths and possibly flow parameters as well, although some groups did not carry out this second calibration stage, because of limited resources, or because their model was considered acceptable without calibration. Thus, the approach adopted for Task 5 was to calibrate the models by adjusting the hydrogeological and transport parameters, rather than by adjusting the initial and boundary conditions for the groundwater composition, as originally envisaged. The initial and boundary conditions for groundwater composition were generally kept fixed throughout the modelling.

The underlying philosophy appeared to be one of ‘re-tuning’ the parameters of the model to find the best, or at least an acceptable, match to the calibration data available at each stage. We think that this does not derive as much support from the geochemical data as might be possible. A demonstration that, without changing the flow parameters, the model provides an acceptable explanation of the geochemical data that are independent of the data used to set up and parameterise the model would probably be taken to provide good support for the model. The fact that, as was done by most of the groups, the flow parameters were changed in order to derive an acceptable match to the geochemical data would probably not be taken to provide as much support for the model.

Further, although the approach adopted is, in a sense, seeking to improve the model at each stage, the improvement is not really quantified. All that can be said is that the revised model matches the additional data. We consider that it would be better to attempt to identify the *range* of models that give reasonably acceptable matches to observations at each stage of increasing information. In this way, the benefits of using geochemical information in terms of reducing the uncertainty would be demonstrated and quantified.

The approaches adopted by the various groups to determining which aspects of their model to change, and by how much, varied. In some cases, these were determined on the basis of the results of a systematic sensitivity analysis, whereas in other cases the decision appears to have been based on expert judgment. We believe that the former approach is better, particularly if the best model at each stage is being sought, because the approach would provide a more justifiable basis for the choices made.

The physical reasonableness of the parameters used has not always been considered. For example, we consider that some of the dispersion parameters used are unrealistically larger or small. If the parameters are unrealistic, the model cannot be considered acceptable, even though it may give an acceptable match to observations.

5.5 Uncertainties

All of the groups described their final calibrated models as giving good fits to data. We would hesitate to describe any of the fits as good. Even allowing for the ±0.1 uncertainty in mixing fractions introduced through the use of the M3 approach, the match is generally poorer than this. Over-optimistic descriptions of the match to data detract from the very real achievements of the groups.

We think that it might have been better if a more quantitative approach had been used, in which the level of agreement between modelled predictions and observations that each group would consider acceptable had been defined and justified a priori. Even if this had not been done, more justification for the accepted levels of discrepancy between the calibrated models and observations would have been useful.

In some cases, models were said to be ‘improved’ by using geochemical data. However, in general the improvement was seldom considered in quantitative terms, which might have been useful. Often, what was meant was simply that the model matched, to some extent, the geochemical data.

As discussed in Subsection 2.2, the approach of the groups has been essentially to seek a single calibrated model that gives an acceptable (in the opinion of each group) match between predictions and observations. We think that it might have been better to try to constrain the uncertainties in the model, that is, to seek to determine the range of models that are consistent with the observations. In this way, the benefits from using geochemical information could be explicitly quantified in terms of the resulting reduction in uncertainty. The uncertainties would be constrained through a combination of sensitivity studies and calibration.

5.6 Presentation

The techniques used by the groups are not always explained clearly in the final reports (as discussed in detail in Section 4). The details of the models, their boundary and initial conditions, and their parameterisation are inadequately explained in some of the reports. In particular, the justification for the choices of parameters to vary during calibration and their variations are not always adequately presented. We think that, in an exercise such as Task 5, it is not sufficient simply to present the final calibrated model. When, as in Task 5, the starting point is well defined, the rationale for changes to the model needs to be explained. A quantitative demonstration of the improvements in the model provides a large part of the justification for the final model. Of course Task 5 was not part of a repository performance assessment for which such justification would be particularly important, but nevertheless we think that some of the reports would have been improved with better explanations.

In the process of calibrating a model, and in order to demonstrate that the model gives an adequate match to observations, it is necessary to make comparisons of the modelled results with observations and in particular to use the directions and inflexions of data trends as well as the values alone.

It is very difficult to present all of the information in a clear and easily understandable manner. Simple comparisons of the evolution of a modelled quantity with the corresponding observations are easy to understand, but many plots are required. Various approaches were adopted by the groups, such as superimposing plots, presenting only a subset of the information, superimposing plots, or more innovative forms of plot. In some cases, so many plots were superimposed that the resulting plots became difficult to interpret. We think that it is best to present as much information as possible, that is, to present comparisons for all of the observation points, although complicated, difficult-to-understand plots should be avoided. One approach that might be adopted to ensure that the reports retain a manageable size would be to present a subset of the comparisons in the report itself, with the full set on an accompanying CD-ROM. We think that the more innovative plots adopted by some groups are rather difficult to understand.

Some of the participating groups calculated backwards pathlines from the observation points and presented plots of these, although this was not done by all of the groups. We think that such plots are a very effective way of helping the reader to understand the modelled changes in groundwater composition, particularly if groundwater composition and travel times are indicated at intervals along the pathlines. However, we recognise that it might not have been practicable for all of the groups to have produced such plots. Estimates of travel times along pathlines from the model boundaries vary from weeks/months to several years, depending of course on the control point and pathline and also on the particular criterion for breakthrough. Not only are these estimated flow times and inferred flow paths effective aspects of presenting results, but they are also important indicators of whether the model domain is an appropriate volume and of how sensitive the model is to the boundary conditions. Another general issue that could be an interesting outcome from modelling is the degree and rate of upconing of more saline water from below the HRL, where the lower boundary condition of the model is not well known.

6 Progress in Integrating Geochemistry and Hydrogeology

We consider that Task 5 has been a significant advance in integrating geochemical information into a groundwater flow and solute transport modelling exercise. This is not an easy objective because hydrogeological and geochemical data have different natures and have different significance for a flow and transport model. Hydrogeological data comprise measures of quantities such as transmissivities (on various length scales), groundwater heads and groundwater inflows to tunnels or boreholes. Measurements of transmissivity provide a suitable basis for setting up a flow model, and measurements of heads and inflows provide suitable data for directly testing a flow model. Geochemical data, which comprise measurements of groundwater composition, are not appropriate data on which to directly base a flow model. Rather they provide information that may be used to constrain either a flow model or transport parameters, in a more indirect manner.

Tangible progress has been made in Task 5 in the development of modelling strategies, in exploring particular approaches to using geochemical information, and not least in identifying some of the issues that affect the credibility of these modelling methods.

We do not know of any comparable study, in terms of size of data set and complexity of both flow system and perturbing process, where such a broadly compelling use of geochemical constraints on a flow model has been achieved. There can be no doubt that, given hydraulic and geochemical conditions that are favourable to this type of exercise, the general objective of 'coupling geochemistry and transport modelling' will have an important rôle in future site investigations.

The achievement of Task 5 can be put in the context of what has been done in previous investigations for repository sites. An integration of geochemical data into the evaluation of a groundwater flow model for the Wellenberg site in Switzerland was an important forerunner of this type of exercise, though it was a more qualitative and conceptual comparison using smaller datasets for hydrogeology and geochemistry (Vomvoris et al., 1999). Other studies, also presented in the NEA/SKB Workshop on the 'Use of Hydrogeochemical Information in Testing Groundwater Flow Models' at Borgholm Sweden in 1997, also had more limited scope. For example, geochemical mass balance and isotopic data were used to constrain flow paths and hydrodynamic travel times (Pitkänen et al., 1999), palaeoclimatic interpretation of $\delta^{18}O$, $\delta^{2}H$ and ^{14}C data were used to constrain travel times (Gascoyne et al., 1999; Schelkes et al., 1999), and chemical distinctions between groundwater masses were used to develop a more complex 3-dimensional representation of the evolution of a groundwater system over time (Corbet, 1999).

It is important to note that the previous case studies indicated above concerned the construction and testing of flow models for undisturbed systems that are either at natural steady state or at least are only undergoing palaeohydrogeological changes over very long timescales. In contrast, Task 5 addressed changes with a much shorter time scale (of order years) resulting from a well-defined perturbation to the groundwater system - the construction of the HRL tunnel. This distinction may have important implications for the potential use of the methodologies developed in Task 5.

It is likely that measurements carried out before and during construction of a tunnel, or other underground facility such as a mine, (or carrying out of a long-term pump test) provide, in a sense, the best data to test a groundwater flow and transport model. Such measurements would provide more data (for a given number of boreholes), in that they would provide data both about the initial conditions (corresponding to the undisturbed system) and the transient response due to the tunnel construction. Changes due to a tunnel or mine are larger than for other experiments, because the inflows to a tunnel or underground facility would be larger than for other experiments.

On the other hand, measurements for an undisturbed system alone can generally only supply data about the conditions at one time (given the timescale for changes to the system). Therefore, geochemical data for an undisturbed system could not be used to test a model as stringently as geochemical data obtained before and during construction of a tunnel. In such a case, using geochemical data in a model test would usually require an interpretation of palaeohydrogeology, i.e. of groundwater conditions at some time in the past.

The differences in groundwater composition that are effectively compared in an analysis of undisturbed conditions or of natural long-term evolution of a groundwater system may be much smaller than the changes occurring as a result of construction of a tunnel. This may have implications for the use of the M3 approach in particular because of the additional uncertainty introduced by the approach (see Section 3), which makes it difficult to assess the implications of small changes.

Further, it may be simpler to interpret the changes resulting from tunnel construction, because the time scales involved may be so short that the dominant process determining the changes in groundwater composition is mixing (which was the underlying assumption for most of the analyses carried out for Task 5) rather than reaction, because the timescales for water-rock interactions are long. This may be part of the reason why the approach to integration in Task 5 worked as well as it did. The approaches used would probably not be as successful if applied to data for an undisturbed system.

However it should also be noted that testing and calibrating a groundwater flow and transport model by comparison with data obtained during construction of a tunnel may not be testing the aspects of the model that would be most important in simulating the flow and transport from a repository post-closure, when conditions might be much closer to undisturbed natural conditions. The flow paths that are important during tunnel construction might not be the same as those that would be important after repository closure. Therefore calibration of the model for the former conditions might not constrain the aspects of the model that are important post closure, or provide much confidence that the model can represent behaviour post closure. In order to address this issue it would be necessary to determine those aspects and parameters of the model that are most important for post closure behaviour, and then determine the extent to which the available information constrains these aspects and parameters. This did not form part of Task 5 but is addressed within Task 6 of the Äspö Modelling Task Force.

A particular feature of Task 5 has been the use of the M3 approach to process geochemical information and thus deliver a more easily visualised and arguably simpler digest of a large and complex hydrochemical data set. This has been an advantage in one sense and a disadvantage in another sense. It has been an advantage in that all the participants used the same set of processed hydrochemical information, i.e. the grid of M3 mixing fractions prior to tunnel construction and the M3 mixing fractions in monitored inflows. It has been a disadvantage in that the alternative outcomes of using information processed by M3 and raw hydrochemical data for conservative species have not been compared by all participants. Fortunately, several modelling groups have evaluated different approaches for using hydrochemical data: such as the 'chemical components' approach, geochemical mixing-reaction modelling (PHREEQC) along discrete flow lines, and transport of individual species rather than mixing fractions.

There is not a single 'best' approach that will always be successful either in terms of model constraints that are tractable for the flow modellers or in terms of demonstrable credibility for potential critics. We have strong reservations about some of the assumptions and simplifications that have been implicit in the way that M3 has been used in Task 5 beyond its original purpose as a data visualisation tool. We do not support the idea that using M3 in the mixing and transport model gets 'additional information' beyond that derived from using one or two conservative species alone. A sound conclusion from Task 5 has to be that the most appropriate approach, and the optimum data in terms of chemical and isotopic parameters and density (space and time) of these data, must be assessed for each individual system, whether it is a perturbation experiment (i.e. Underground Rock Laboratory or long-term pumping test) or a palaeohydrogeological interpretation. These considerations must take account of the assumptions that are involved in the interpretative models for groundwater flow and geochemistry.

A key feature of Task 5 has been the availability of the large data set, both hydrogeological and geochemical, for the Äspö site, and specifically from monitoring during and after construction of the HRL tunnel. The numerical groundwater flow model that has been developed over many years by the SKB groups at Äspö was the foundation of Task 5. The structure, geometry and parameterisation of the site-scale model are at an advanced stage of calibration and refinement because of the preceding modelling exercises and experiments, notably Task 3 of the Task Force. It may only have been because the hydrogeology was so well defined, and there were so many data, that Task 5 worked as it did. Had there been fewer geochemical and hydrogeological data (including information on the palaeohydrogeology of the Äspö site), the exercise might have been more problematical in terms of achieving credible fits between model and data. On the other hand, it might then have provided an evaluation of the approach under conditions perhaps more appropriate to a typical site characterisation.

Another key factor is the long development of knowledge about the structural model. Perhaps because of this reason, the studies in Task 5 did not seek to use the data to rule out alternative interpretations or models, although this is one of the potential uses of geochemical data. More effort might perhaps have been put into attempting to use the data in this fashion.

Task 5 has involved an impressive amount of work that has focused the capabilities of a range of diverse models on a single exercise. Nine modelling groups have participated, and contributed to the overall result with outputs from many different models and approaches. The Task has been carried out over a period of around 3 years and, despite the varying objectives and resources of individual organisations, the Task has remained a coherent effort due to the management by the Task Force delegates and the SKB group.

In final summary, the studies carried out for Task 5 have provided a clear demonstration that geochemical data can be used to improve models, in the general sense that the models would be shown to fit a wider range of data and would therefore be more reliable and credible. However, the studies have also been limited in the sense that they have not demonstrated clearly the potential use of such data to reduce uncertainties in the characterisation of a groundwater system or to limit the number of alternative conceptual models.

Part 2:

Transport of M3 Mixing Fractions

C P Jackson

1. Introduction

There are potentially considerable benefits in integrating geochemical models with models of groundwater flow and transport model at a site. Such flow and transport models would be needed, for example, as part of an assessment of the performance of an underground repository for radioactive waste. The use of geochemical information in the development of the flow and transport models:

(a) can improve understanding of the flow system;
(b) has the potential to lead to more realistic and more robust models;
(c) is likely to improve the confidence of others in the models, which is very important for a repository performance assessment.

However, there may be difficulties in integration of geochemical information into hydrogeological models. Geochemical information consists of measured concentrations for various groundwater constituents at various locations. The concentrations are the results of mixing and reactions between groundwaters with different compositions and reactions between the groundwater and the rock through which it flows. The resulting patterns in the distribution of the different constituents may be complex and difficult to interpret. Further, it may not be easy to present the information in a readily understandable form, which would be very important for a repository performance assessment.

In order to address these issues, a new approach to the interpretation of geochemical information has been developed within the Swedish radioactive waste disposal programme. This approach, the Multivariate Mixing and Mass-balance (M3) approach (Laaksoharju et al., 1999; Laaksoharju and Wallin, 1997; Rhén et al., 1997c), which is described in Section 2, is based on interpreting the observed groundwaters primarily in terms of mixing of a small number of 'reference waters', with the deviations of the compositions from the results of ideal mixing being interpreted as due to reactions. This approach differs from the standard approach to interpretation of geochemical information, in which the observed groundwater compositions are interpreted primarily in terms of reactions. A particular benefit of the M3 approach is that it enables complicated geochemical information to be presented in a form that is probably much more readily understandable by those without geochemical expertise. The approach therefore potentially provides a powerful framework for integrating hydrogeology and geochemistry.

The M3 approach has been used in studies carried out for Task 5 (Wikberg, 1998) of the Äspö Task Force. At Äspö, an underground Rock Laboratory was constructed some years ago as a research facility to support the Swedish radioactive waste disposal programme. The aim was to assist in the development and testing of approaches to be used in characterising a suitable site for a repository for radioactive waste, and in demonstrating the feasibility of safe disposal of waste in such a repository. The Äspö Task Force was set up to provide a forum for the international organisations supporting the Hard Rock Laboratory to interact on the topics of conceptual and numerical modelling of groundwater flow and transport in fractured rock. Task 5 specifically addresses the integration of geochemical and hydrogeological modelling. It is based around modelling of (i) the flow of waters into the underground tunnel that forms the Hard Rock Laboratory, and (ii) the chemistry of the inflowing waters, using data obtained during the construction of the Hard Rock Laboratory.

Much of the work carried out on Task 5 was ultimately based on the M3 approach. In most analyses, the M3 mixing fractions (that is, the fractions of a groundwater that correspond to the various reference waters) were assumed to obey the standard advection-dispersion equation (ADE). This is the equation that is obeyed by the concentrations of the groundwater constituents in the absence of reactions. However, (see Section 3) if there are more than three reference waters, the mixing fractions do not obey the standard ADE, but a slightly modified equation containing an additional term, which does not have the form of any of the usual terms in the ADE. This is because the relation between the mixing fractions and the concentrations of the groundwater constituents is non-linear if there are more than three reference waters.

Therefore, use of the standard ADE for the mixing fractions will have introduced errors into the modelling. It is not immediately apparent whether these errors are small enough to be considered negligible, in comparison with, for example, the other approximations made in the M3 approach. The additional term in the equation for the M3 mixing fractions is generally small except in the regions where groundwater with different compositions are mixing. However, these are the regions of particular interest.

This issue is particularly important because the M3 approach may also be used in work to be carried out for the sites in Sweden chosen for investigation as potential candidate sites for a deep repository for radioactive waste. Therefore, a study of the issue was undertaken. The approach adopted was to consider various cases in which flowing groundwaters of different compositions mix and to compare mixing fractions calculated on the assumption that they obey the standard ADE with mixing fractions calculated from the transport equation that they really satisfy. The latter mixing fractions were actually determined by calculating the evolution of the groundwater constituents, which obey the standard ADE and then evaluating the mixing fractions, rather than by explicitly calculating the evolution of the mixing fractions using the equation that they satisfy. The calculations were carried out for cases in which there are simple analytical solutions to the transport equations. This allowed the study to be carried out using a simple spreadsheet, rather than requiring the use of a finite-difference or finite-element program to carry out the transport calculations.

The results of the study are presented in this report. In Section 2, the M3 approach is summarised. In Section 3, the transport equations that the mixing fractions really obey are discussed. In Section 4, the simple analytical solutions to the ADE that were used in the study are outlined. In Section 5, the quantitative comparison of the mixing fractions calculated in the different ways is presented. Finally, in Section 6, the implications of the study are discussed.

2. The M3 Approach

The M3 approach consists of four main steps (Laaksoharju et al., 1999; Laaksoharju and Wallin, 1997; Rhén et al., 1997c). The first step is a principal component analysis of the measured compositions of the groundwater samples. Principal component analysis (see for example, Davis (1973)) is a standard technique of multi-variate analysis. If the composition of each sample is taken to correspond to a point in a multi-dimensional space with a coordinate for each constituent, principal component analysis consists essentially of seeking a rotation of the coordinates to determine new coordinate axes (directions of principal components) such that the spread of the projection of the cloud of points corresponding to the samples onto the first new axis is as large as possible; and given this, the spread of the projection onto the second new axis is as large as possible, and so on (see Figure 2-1). The principal component analysis is actually carried out in terms of standardised values, $\hat{c}_\alpha$, of the measurements of the concentration of the different groundwater constituents, which are given by

$$\hat{c}_\alpha = \frac{c_\alpha - m_\alpha}{s_\alpha} \quad , \tag{1}$$

where

c_α is the concentration of the α'th groundwater constituent;
m_α is the mean of the measurements of c_α;
s_α is the standard deviation of the measurements of c_α.

The use of standardised values enables quantities that have different units or different orders of magnitude to be taken into account in the analysis on the same footing. The principal components, P_α, are linear combinations of the standardised concentrations of the groundwater constituents:

$$P_\alpha = \sum_\beta a_{\alpha\beta} c_\beta \quad , \tag{2}$$

where $a_{\alpha\beta}$ are constant coefficients (called 'loadings' in principal component analysis).

In many cases of interest, the cloud of points only has a large spread in two (or perhaps three) orthogonal directions, that is the new axes. Effectively the quantities corresponding to the remaining orthogonal directions are correlated with the quantities corresponding to the first two (or three) directions. It should be remembered that the quantity corresponding to each new axis is not one of the original groundwater constituents, but a particular linear combination of these. In this case, the bulk of the information in the original measurements can be conveniently presented, without significant loss of information, in the projection of the cloud of points onto the first two (or three) new axes. In this way, most of the information contained in the measurements of many different groundwater constituents can be summarised in terms of only (or three) quantities: the first two (or three) principal components.

Henceforth, for clarity of presentation, the case in which two principal components are adequate to summarise the geochemical information will be discussed. The modifications to deal with the case in which it is better to use three (or even more) principal components are straightforward. For convenience, the projection of the scatter plot onto the first two principal components will be referred to henceforth as the M3 plot.

The second step in the M3 analysis is to identify a small number of reference waters. This is done on the basis of the M3 plot, supported by physical and geochemical understanding of the groundwater flow system at the site of interest. The aims are that the points in the M3 plot corresponding to the reference waters should form the corners of a polygon, which contains all the points in the M3 plot corresponding to the observed groundwater compositions at the site, and that the reference waters should correspond to water compositions that have physical and geochemical significance for the site, taking into account the fact that all water compositions will subsequently be approximated as mixtures of the reference waters. Figure 2-2 illustrates a possible choice of reference waters in a particular case (based on data from Äspö, see below). The reference waters are not uniquely determined by the scatter plot, but depend, to some extent, on the judgment of the analyst.

The third step in the M3 approach is to determine for each sample a mixture of the reference waters that would have the same first two principal components as the sample. If there are only three reference waters, then this can only be done in one way. In this case, the fraction of each reference water in the mixture is given by the ratio of the area of the triangle whose corners correspond to the two other reference waters and the sample to the area of the triangle whose corners correspond to the reference waters (see Figure 2-3).

However, if there are more than three reference waters (in a case in which the analysis is being carried out on the basis of the first two principal components), then the mixing fractions are not uniquely determined. For example, if there are four reference waters, the point at the intersections of the lines between the pairs of points corresponding to the reference waters that are diagonally opposite one another in the M3 plot could be expressed as a mixture of one of the two pairs of diagonally opposite reference waters, or as mixture of the other pair of reference waters, or as various mixtures of all four reference waters (see Figure 2-4).

In order to deal with this potential ambiguity, a definite prescription for determining the mixing fractions is given as part of the M3 methodology. The point in the M3 plot corresponding to a mixture of the reference waters in equal proportions is determined. The polygon formed by the points corresponding to the reference waters is subdivided into triangles by lines joining the corners to the central point (see Figure 2-5). Then, the mixing fractions for a particular sample are determined as follows. The triangle in which the point in the M3 plot corresponding to the sample lies is determined. Fractions of the three corner waters (two reference waters and a mixed water corresponding to the central point) that would give a mixture with the same first two principal components as the sample are determined using the prescription for three reference waters described above. Finally, the mixing fractions for the original reference waters are calculated. This gives a unique prescription for the mixing fractions. In order to recognise the ambiguity, a prescription for the uncertainty in the mixing fractions is also given. For example, for the groundwaters at Äspö, the uncertainty was estimated to be ±0.1 (Rhén et al., 1997c), and it was also stated that mixing fractions of less than 0.1 have no significance.

The fourth step in the M3 approach is to determine, for each groundwater sample, the deviations of the concentrations of the various groundwater constituents from the values that they would have as a result of mixing the reference waters in the fractions given by the calculated mixing fractions. These deviations are interpreted as the result of reactions.

3. Transport Equations

3.1 Advection-dispersion Equation (ADE)

In the absence of reactions, and away from possible sources or sinks, the concentration of a solute dissolved in groundwater flowing through a porous medium is normally considered to obey the so-called scalar-transport or advection-dispersion equation (ADE):

$$R\phi \frac{\partial c}{\partial t} + \mathbf{q} \cdot \nabla c = \nabla \cdot \left[(D_{\mathrm{i}} \mathbf{I} + \phi \mathbf{D}) \cdot \nabla c \right] - \lambda R \phi c \quad , \tag{3}$$

where

c	is the concentration of the solute;
$\mathbf{q}$	is the specific discharge (or Darcy velocity);
D_{i}	is the intrinsic diffusion coefficient (which depends on the solute);
$\mathbf{I}$	is the identity tensor;
$\mathbf{D}$	is the dispersion tensor;
R	is the retardation factor;
ϕ	is the kinematic porosity of the medium;
λ	is the decay rate for a radioactive solute.

The components of the dispersion tensor **D** are usually taken to be given by

$$D_{ij} = a_{\mathrm{T}} v \delta_{ij} + (a_{\mathrm{L}} - a_{\mathrm{T}}) \frac{v_i v_j}{v} \quad (i, j = 1, 2, 3), \tag{4}$$

where

a_{L}	is the longitudinal dispersion length;
a_{T}	is the transverse dispersion length;
v_i, v	are the components and magnitude of the transport velocity

$$\mathbf{v} = \frac{\mathbf{q}}{\phi} \quad . \tag{5}$$

(Solute transport in a network of fractures is described by a similar two-dimensional equation in each fracture.)

In almost all cases of regional-scale or repository-scale groundwater flow, the diffusion term in Equation (3) is negligible compared to the dispersion term. Then, if there are several non-sorbing and non-decaying groundwater constituents, their concentrations, c_α, all obey the same transport equation:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot \left[\mathbf{D} \cdot \nabla c \right] \ , \tag{6}$$

This is linear in the concentration, and the coefficients are the same for the concentrations of all the groundwater constituents, and so any linear combination

$$c = \sum_{\alpha} a_{\alpha} c_{\alpha} \ , \tag{7}$$

of the concentrations, where a_α are constants, obeys the same equation. In particular, the principal components (which are given by Equation (2)) also obey the same equation.

However, if some of the constituents are sorbing or if reactions occur, then the general linear combination of concentrations given by Equation (7) does not obey such a simple equation as Equation (6). If chemical reactions taken place in the groundwater, or between the groundwater constituents and the rock, then transport equations for all the significant compounds in the system have to be developed. These equations are similar to Equation (3), but include additional source and sink terms that represent the production and destruction of the various compounds as a result of reactions. The source and sink terms are generally non-linear. Typically they involve products of powers of the concentrations of the reactants. As a result of the non-linearity, again the general linear combination of concentrations given by Equation (7) does not obey the simple ADE of Equation (6).

3.2 Transport Equation for Mixing Fractions

The essence of the issue discussed in this report is that the M3 mixing fractions are not, in general, linear combinations of the concentrations of the groundwater constituents, and as a result, the mixing fractions do not obey the simple ADE of Equation (6), even in the case without sorption, decay or reaction. This can be easily seen, as follows. In the case in which there are more than three reference waters (and two principal components are used), the relationship between the mixing fractions and the concentrations of the groundwater constituents is not linear, but piecewise linear. The relationship is linear within each of the triangles into which the reference polygon has been subdivided (see Section 2), but the coefficients are different within each triangle. This is because within the different triangles, the groundwater is expressed as mixtures of the two reference waters and the central mixed water corresponding to the corners of the triangle, and the reference waters in question are different for each triangle.

If the mixing fractions, M_α are general non-linear functions

$$M_{\alpha} = M_{\alpha}(c_1, c_2, \Lambda) \ , \tag{8}$$

of the concentrations of the groundwater constituents, c_α, the equations satisfied by the mixing fractions can be determined as follows. From Equation (8),

$$\frac{\partial M_\alpha}{\partial t} = \sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\frac{\partial c_\beta}{\partial t} \quad , \tag{9}$$

$$\frac{\partial M_\alpha}{\partial x_i} = \sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\frac{\partial c_\beta}{\partial x_i} \quad , \tag{10}$$

and from equation (10)

$$\frac{\partial^2 M_\alpha}{\partial x_i \partial x_j} = \sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\frac{\partial^2 c_\beta}{\partial x_i \partial x_j} + \sum_\beta \sum_\gamma \frac{\partial^2 M_\alpha}{\partial c_\beta \partial c_\gamma}\frac{\partial c_\beta}{\partial x_i}\frac{\partial c_\gamma}{\partial x_j} \quad , \tag{11}$$

Assuming that the groundwater constituents are non-reacting, non-sorbing and non-decaying, their concentrations obey the ADE of Equation (6).
Therefore

$$\sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\left(\frac{\partial c_\beta}{\partial t} + \mathbf{v}\cdot\nabla c_\beta\right) = \sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\nabla\cdot\left[\mathbf{D}\cdot\nabla c_\beta\right] \quad , \tag{12}$$

or, in component notation,

$$\sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\left(\frac{\partial c_\beta}{\partial t} + \sum_i v_i \frac{\partial c_\beta}{\partial x_i}\right) = \sum_\beta \frac{\partial M_\alpha}{\partial c_\beta}\sum_i \sum_j \left(\frac{\partial D_{ij}}{\partial x_i}\frac{\partial c_\beta}{\partial x_j} + D_{ij}\frac{\partial^2 c_\beta}{\partial x_i \partial x_j}\right) \quad , \tag{13}$$

Substituting from Equations (9), (10) and (11), the mixing fractions obey the equations

$$\begin{aligned}
&\left(\frac{\partial M_\alpha}{\partial t} + \mathbf{v}\cdot\nabla M_\alpha\right) \\
&\quad = \sum_i \sum_j \left\{\frac{\partial D_{ij}}{\partial x_i}\frac{\partial M_\alpha}{\partial x_j} + D_{ij}\left(\frac{\partial^2 M_\alpha}{\partial x_i \partial x_j}\right) - D_{ij}\sum_\beta \sum_\gamma \frac{\partial^2 M_\alpha}{\partial c_\beta \partial c_\gamma}\frac{\partial c_\beta}{\partial x_i}\frac{\partial c_\gamma}{\partial x_j}\right\} \\
&\quad = \nabla\cdot\left[\mathbf{D}\cdot\nabla M_\alpha\right] - D_{ij}\sum_i \sum_j \sum_\beta \sum_\gamma \frac{\partial^2 M_\alpha}{\partial c_\beta \partial c_\gamma}\frac{\partial c_\beta}{\partial x_i}\frac{\partial c_\gamma}{\partial x_j} \\
&\quad = \nabla\cdot\left[\mathbf{D}\cdot\nabla M_\alpha\right] - D_{ij}\sum_i \sum_j \sum_\beta \sum_\gamma \sum_\delta \sum_\varepsilon \frac{\partial^2 M_\alpha}{\partial c_\beta \partial c_\gamma}\frac{\partial c_\beta}{\partial M_\delta}\frac{\partial M_\delta}{\partial x_i}\frac{\partial c_\gamma}{\partial M_\varepsilon}\frac{\partial M_\varepsilon}{\partial x_j} \quad ,
\end{aligned} \tag{14}$$

which corresponds to the standard ADE, with an additional term

$$-D_{ij}\sum_i \sum_j \sum_\beta \sum_\gamma \sum_\delta \sum_\varepsilon \frac{\partial^2 M_\alpha}{\partial c_\beta \partial c_\gamma}\frac{\partial c_\beta}{\partial M_\delta}\frac{\partial M_\delta}{\partial x_i}\frac{\partial c_\gamma}{\partial M_\varepsilon}\frac{\partial M_\varepsilon}{\partial x_j} \quad . \tag{15}$$

This term has to be expressed in terms of the M_α, which will involve inverting the relationship between M_α and c_β to express c_β as a (non-linear) function of M_α. Note that $\frac{\partial c_\beta}{\partial M_\delta}$ is just the inverse of $\frac{\partial M_\delta}{\partial c_\beta}$. The additional term of Equation (15) is large in regions where $\frac{\partial^2 M_\alpha}{\partial c_\beta \partial c_\gamma}$ is large, that is in regions where the relationship between M_α and c_β is most non-linear.

In the case of particular interest, in which the mixing fractions are determined using the prescription given in Section 2, the relationship between M_α and c_β is not everywhere differentiable, and Equation (14) has to be interpreted in a generalised sense. However, it is clear that the mixing fractions do not obey the standard ADE.

4. Analytic Solution to the ADE

For the purpose of this study, it was necessary to compare mixing fractions calculated in two ways:

(i) on the basis that the mixing fractions obey the standard ADE, which is not correct (see subsection 3.2);
(ii) from the actual transport equation that they satisfy (see subsection 3.2).

The required calculations could have been carried out using finite-difference or finite-element numerical techniques. However, it was more convenient to use simple analytical solutions to the ADE. This meant that the calculations could be carried out using a spreadsheet.

In fact, all the calculations were carried out using analytical solutions to the ADE based on what is probably the simplest such solution corresponding to the mixing of groundwaters with different initial concentrations. This solution is

$$c = c_0 + \tfrac{1}{2}(c_1 - c_0)\,erfc\left(\frac{x - x_0 - vt}{2\sqrt{Dt}}\right) \quad . \tag{16}$$

This describes the evolution over time of an infinite one-dimensional system in which initially (at t=0) part of the domain (x>x_0) is at concentration c_0 and part (x<x_0) is at concentration c_1. A mixing zone develops between the regions at different concentrations. The zone moves with the transport velocity (v) and broadens over time (see Figure 2-6).

Although the solution given in Equation (16) corresponds to a case that might be thought to be very idealised, in that, in particular, it corresponds to mixing in an infinite domain, with a very specific initial condition, the solution of Equation (16) was considered to be the best for the purposes of the current study. Analytical solutions can be developed (using Laplace transform techniques) for other cases, such a semi-infinite domain. However, these solutions are much more complicated, but have no particular advantages for the purpose of this study. In the vicinity of mixing zones, their behaviour is similar to that of the simple analytic solution of Equation (16).

With appropriate interpretation of parameters, Equation (16) also gives, to a good approximation, the steady-state distribution of concentration in a two dimensions for a half space in which part of the boundary of the half space is held at concentration c_0 and the remainder is held at concentration c_1 (see Figure 2-7). (The approximation neglects dispersion in the direction parallel to travel, which is reasonable at steady state because the gradients in this direction are generally small.).

5. Comparison of the Mixing Fractions Calculated in Different Ways

As discussed in the Introduction and Section 3, the basic issue of concern in this study is that the M3 mixing fractions do not obey the standard ADE, although it was assumed that they do in much of the analysis that was carried out for Task 5 of the Äspö Task Force, for example. In the current study, the size of the errors resulting from the assumption that the mixing fractions obey the standard ADE was examined. The approach adopted was to compare mixing fractions calculated on the assumption that they obey the standard ADE with mixing fractions calculated from the transport equation that they really satisfy. This was done for one-dimensional cases involving the development of the mixing zone between two regions with different groundwater composition, as in Section 4.

In order to make the study as relevant as possible to the studies carried out for Äspö Task 5, only compositions that could, in principle, correspond to groundwaters at Äspö were selected. That is, only compositions corresponding to points within the polygon defined by the reference waters in the M3 plot used for Task 5 were selected (see Figure 2-8). The essence of the issue under discussion is that mixing corresponds to following the straight line between the points, but the mixing fractions do not vary linearly along this line. A linear variation of the mixing fractions may correspond to a line composed of several segments (see Figure 2-8).

The mixing fractions calculated on the assumption that they obey the ADE were obtained from the simple analytic solution to the ADE given by Equation (16). The mixing fractions calculated from the transport equation that they really satisfy were not directly calculated from this transport equation (which was never explicitly determined). Instead, one of the following approaches was adopted:

A. The compositions of the two groundwaters mixing were specified in terms of the first two principal components and the development of mixing zones for the principal components was modelled using the analytic solution of Equation (16). (As discussed in Section 3, neglecting reactions and sorption (and decay), which are fundamental assumptions underlying the use of mixing fractions, the principal components obey the standard ADE). Then the mixing fractions were evaluated from the calculated principal components in the mixing zone.

B. The compositions of the two groundwaters mixing were specified in terms of the concentrations of the groundwater constituents and the development of mixing zones for these concentrations was modelled using the analytic solution of Equation (16). (As discussed in Section 3, neglecting reactions and sorption (and decay), which are fundamental assumptions underlying the use of mixing fractions, the concentrations of the groundwater constituents obey the standard ADE.) Then principal components were calculated in the mixing zone, and then the mixing fractions were evaluated from the calculated principal components.

In the absence of reactions and sorption, both of these approaches give the results that would be obtained by solving the equations actually obeyed by the M3 mixing fractions, which are really determined by approach **B**, anyway. As discussed in Section 3, in the absence of reactions and sorption (and decay), the principal components and the concentrations of the groundwater constituents satisfy the standard ADE. In this case, using all the principal components is equivalent to using all of the concentrations. For approach **A**, only the first two principal components were used. Effectively, this is equivalent to approach **B** with the remaining principal components, which do not affect the M3 mixing fractions, being ignored. The main difference between the approaches is not in the underlying transport equations, but in the variation of the weight effectively ascribed to points in the M3 plot, which is significant for the Monte-Carlo studies carried out (see below). Approach **B** also has the benefit that it is the only approach that is defined in the case in which sorption or reactions occur. It can therefore be used to examine the impact of these processes on the mixing fractions.

The study undertaken can be divided into several parts:

5.1 Deterministic Study

First, a deterministic study was carried out, in which the comparisons of the mixing fractions calculated in the different ways were made for a few manually selected groundwater compositions. This study gave some interesting results. A typical comparison between the mixing fractions calculated assuming that they obey the standard ADEs and using approach **A** above is shown in Figure 2-9. The mixing fractions calculated on the assumption that they obey the ADE are generally fairly close to the mixing fractions calculated from the equations that they really satisfy. In the case shown, the maximum difference between the corresponding mixing fractions is only about 0.12. In cases in which the compositions of the groundwaters mixing correspond to points that lie in the same triangle within the M3 polygon, the differences are of course zero (because the relationship between the mixing fractions and the principal components, or the concentrations of the groundwater constituents, is linear within a single triangle).

However, in some cases the difference can be much larger. In fact for the first case considered, in which one of the mixing waters had the composition of the Brine reference water and the other had the composition of the Meteoric reference water, the maximum difference was about 0.43! This might be considered surprising, since it might perhaps be thought that the maximum error in one of the mixing fractions would be 0.25, corresponding to the ambiguity between mixing two of the reference groundwaters at opposite corners of the M3 polygon, or all four reference groundwaters, to give the composition of a point in the middle of the M3 plot.

However, it must be noted that the central point introduced into the M3 polygon, is generally not half-way between two opposite corners of the polygon. Rather the central point has coordinates that are the averages of the coordinates of all four of the corners of the polygon. In the present case of the M3 analysis for the groundwaters at Äspö, three of the reference waters (Glacial, Meteoric and Baltic) have similar first principal components. The central point therefore has a first principal component that is much closer to the first principal component of these three reference waters than it is to the first principal component of the fourth reference water (Brine). Therefore, in comparing the mixing of waters with compositions corresponding to the Brine and Meteoric reference waters, calculated on the assumption that the mixing fractions obey the standard ADE and the on the basis of the equations that they really satisfy, the comparison is much closer to the comparison of (a) and (c) in Figure 2-10, rather than a comparison of (a) and (b). Therefore, a discrepancy of about 0.43 is not surprising.

Another interesting result was that in some cases, although the mixing fractions calculated on the assumption that they obey the standard ADE vary monotonically over the mixing zone, the mixing fractions calculated from the equations that they really satisfy do not all vary monotonically. For example, as in Figure 2-11, one of the mixing fractions may, on crossing through the mixing zone, first increase and then decrease to a lower value than its initial value. The particular significance of this issue is that it means that one cannot reliably infer the ultimate direction of change from the initial direction of change. This is particularly important in the comparison of the results of numerical models with experimental observations to try to validate the models, as in the studies carried out for Äspö Task 5. Such comparisons are usually considered as providing some support for the model if the predicted direction of change is right, even if the rate of change is not well predicted. However, the results discussed show that for models that are based on the assumption that the mixing fractions obey the standard ADE the initial direction of change is not reliably given by the model, and so great care must be taken in inferring support for a model on the basis that the predicted direction of change matches that observed.

5.2 First Monte-Carlo Study

The comparisons discussed above illustrate the worst aspects of calculating the mixing fractions on the basis that they obey the standard ADE. However, this behaviour was obtained in particular cases for the mixing of groundwaters with selected groundwater compositions. It is also very important to examine the errors that are made, on average, as a result of assuming that the mixing fractions obey the standard ADE. In order to do this, two Monte-Carlo studies were undertaken in which the mixing fractions in the mixing zone calculated on the assumption that they obey the standard ADE were compared with mixing fractions calculated from the equations that they actually obey.

In the first Monte-Carlo study, approach **A** was used to calculate the correct mixing fractions. For each realization of the Monte-Carlo study, values of the first two principal components for the two mixing groundwaters were selected at random within the M3 polygon for the groundwaters at Äspö with a uniform distribution over the polygon. This was actually done by generating random values of the first two principal components with uniform distributions between their minimum and maximum values within the polygon, and then discarding combinations that correspond to a point outside the polygon.

The mixing fractions in the mixing zone were then calculated on the assumption that the mixing fractions obey the standard ADE and on the basis of the equations that they actually obey, using approach **A** described above. The following measures of the discrepancy between the mixing fractions calculated in the two ways for the realization were then evaluated:

(a) the maximum discrepancy for each mixing fraction;
(b) the mean of the maximum discrepancy over the mixing zone. (For definiteness in calculating the average over the mixing zone, for the parameters used, the mixing zone was taken to cover the region between 99.9% and 0.4% mixing of the incoming groundwater.)
(c) the number of mixing fractions for which the initial direction of change is oppositely directed to the ultimate direction.

The averages of these measures over all the realizations were then calculated. The results for a suite of 100 realizations are as follows:

(a) the average of the mean error in a mixing fraction is about 0.01;
(b) the average of the maximum error in a mixing fraction is about 0.04;
(c) the maximum of the maximum error in a mixing fraction is about 0.35;
(d) the average number of mixing fractions that have an incorrect initial direction of change is about 0.75. That is, on average, slightly fewer than one mixing fractions in each realization potentially has the wrong direction of change.

Of these results, all except (c) are well-converged statistically, in that a second suite of realizations gave very similar results. (c) was still reasonably well–converged, but did vary by more between the two suites of realizations, as would be expected.

5.3 Second Monte-Carlo Study

The second Monte-Carlo study was similar to the first, except that approach **B** was used to calculate the mixing fractions on the basis of the equations that they really satisfy, and for each realization the compositions of the mixing groundwaters were not determined by randomly selecting values of the first two principal components, but by randomly selecting values of the concentrations of the groundwater constituents, still in such a way that the mixing groundwaters lie within the M3 polygon for the groundwaters at Äspö. This was done by selecting values of the concentration of each groundwater constituent with a uniform distribution between its maximum and minimum, and then discarding combinations that correspond to a point outside the polygon. The same measures of the discrepancies between the mixing fractions calculated in the different ways were then calculated as in the previous Monte-Carlo study. As indicated above, the difference between this study and the previous one is that a different weight is effectively ascribed to points in the M3 polygon.

The results of this study are as follows:

(a) the average of the mean error in a mixing fraction is about 0.005;
(b) the average of the maximum error in a mixing fraction is about 0.015;
(b) the maximum of the maximum error in a mixing fraction is about 0.13;
(c) the average number of mixing fractions that have an incorrect initial direction of change is about 0.5.

Of these results, all except (c) are well-converged statistically, in that a second suite of realizations gave very similar results. (c) was still reasonably well–converged, but did vary by more between the two suites of realizations, as would be expected.

5.4 Effects of Sorption

Finally, in order to begin to examine the effects of reactions, a study was undertaken in which one or more of the groundwater constituents were taken to be retarded by sorption. The constituents in question were those that might be expected to react with the rock. The effects were much as would be expected. If a retarded constituent was present at significant concentration in the water moving into the domain, it was effectively left behind and stripped out of the groundwater in the zone where the unretarded constituents mix. As a result, there were substantial errors in the mixing fractions calculated on the basis of the assumption that the mixing fractions obey the standard ADE.

6. Discussion

This study has shown that although the mixing fractions do not actually obey the standard ADE, the error resulting from assuming that they do is on average fairly small. The average error is probably smaller than the typical error resulting from experimental errors in the measurement of the concentrations of the groundwater constituents. Therefore, this study provides some support for the use of the assumption that the mixing fractions obey the standard ADE as an approximation. It is recommended, that if the approach is used, it be made clear that it is only an approximation.

It should be noted that the error could be large in particular cases. It should also be noted that the initial direction in which a mixing fraction is predicted to change on passing through a mixing zone may be incorrectly predicted. On average this occurs for slightly less than one of the mixing fractions. This means that great care must be taken in inferring support for a model on the basis of a match between the predicted and observed directions of change, if the mixing fractions have been calculated using the assumption that they obey the standard ADE.

The quantitative measures of the errors were obtained for mixing of two groundwater compositions that were, in some sense randomly selected from the groundwater compositions at Äspö. However, many experiments at the site would involve the mixing of groundwaters that are much closer in composition than randomly selected groundwaters. For such experiments, the errors would be much smaller than those quoted.

The results presented were obtained for the groundwaters at Äspö. However it is clear from the study that similar results would be expected for groundwaters from a different site. The underlying issue is basically the result of the ambiguity inherent in describing a system characterised by only two principal components in terms of four (or more) reference waters. The M3 approach provides a prescription for removing the ambiguity, but the issue remains. A mixture of groundwaters will not in general give a groundwater whose mixing fractions (obtained from the M3 prescription) correspond to a mixture of the mixing fractions for the original groundwaters.

The values of the error measures would depend on the site. If the approach of calculating the mixing fractions on the basis of the assumption that they obey the standard ADE is to be used for a different site from Äspö, it is recommended that a study similar to that reported here is carried out to quantify the errors.

As indicated, the study has provided some support for calculating the mixing fractions on the basis of the assumption that they obey the standard ADE. However, there are no real benefits from so doing. Although the use of the M3 mixing fractions for presenting geochemical information has considerable benefits in terms of presenting the information in a readily understandable form to those who are not geochemists, it is not necessary to derive the mixing fractions on the basis of the (incorrect) assumption that they obey the standard ADE in order to present the geochemical information using the mixing fractions. Instead, approaches that are more rigorous can be used to model the mixing of different groundwaters (see below), and then the mixing fractions calculated and used to present the results of the modelling.

Further, there are significant disadvantages to calculating mixing fractions on the basis of the assumption that they obey the standard ADE:

(a) Although the resulting error is on average small, the error can be substantial in particular cases, as discussed above. The use of the assumption introduces additional uncertainty into the modelling. This makes it more difficult to ascribe significance to comparisons of the results of modelling with experimental data. Significance can only be attached to differences that are bigger than the uncertainties (quoted as ±0.1 for the groundwaters at Äspö (Laaksoharju et al., 1999; Laaksoharju and Wallin, 1997; Rhén et al., 1997c), but see the discussion above). Thus, in principle, a model might not be rejected that would have been rejected had an approach with smaller uncertainties been adopted. This therefore reduces the confidence in models that are considered to match the available data within the uncertainties. This may be particularly important for cases in which the changes in composition are small, which is likely to be the case in many practicable experiments.

(b) The approach of calculating the M3 mixing fractions on the basis of the assumption that they obey the standard ADE is actually more computationally costly than an alternative approach that is also more rigorous. Although there are more of them, the mixing fractions contain no more information than the first two principal components, because they are derived from the latter. As discussed in subsection 3.1, if the assumption, which underlies the use of mixing fractions, is made that there are no reactions or sorption, then the first two principal components actually do obey the standard ADE (unlike the mixing fractions). The computational cost of calculating the first two principal components using the standard ADE is considerably less than the computational cost of calculating the mixing using the standard ADE. For example, for the groundwaters at Äspö, the computational cost of calculating the former approach is about half that of the latter, because there are four mixing fractions.

(c) It is considered that the approach of calculating the M3 mixing fractions on the basis of the assumption that they obey the standard ADE is likely to be viewed with some suspicion by those not familiar with the approach. This is particularly undesirable for an approach that may be used in work undertaken in support of characterisation and performance assessments for a potential site for a repository for radioactive waste.

In summary, the approach of calculating the mixing fractions on the basis of the assumption that they obey the standard ADE has nothing to recommend it, but introduces additional uncertainties, is more costly than an alternative, and is likely to be viewed with suspicion by those unfamiliar with it. It is therefore suggested that, in cases in which reactions and sorption can be neglected, the alternative approach of calculating the first two principal components using the standard ADE would be preferable. This approach would be more defensible and computationally cheaper.

In the case in which reactions, or sorption are not neglected, the only justifiable approach is to calculate the concentrations of the groundwater constituents from the transport equations that they satisfy, with appropriate sorption of reaction terms. This approach may also be a suitable approach in the case in which reactions and sorption can be neglected. The approach would be rigorous in such cases, and it would be an approach expected by hydrogeologists and geochemists unfamiliar with the M3 approach. As such it would be unlikely to be viewed with suspicion. However, the approach has a greater computational cost than either of the alternatives: making the calculations on the basis of the assumption that the mixing fractions obey the standard ADE, or determining the first two principal components using the standard ADE.

Finally, it should be emphasised that the use of the M3 mixing fractions to present geochemical information has considerable benefits in terms of presenting the information in a readily understandable form to those who are not geochemists. It is therefore recommended that whatever approach is adopted for modelling the mixing of groundwaters, the results are presented using the M3 mixing fractions, as well as in terms of the concentrations of the groundwater constituents.

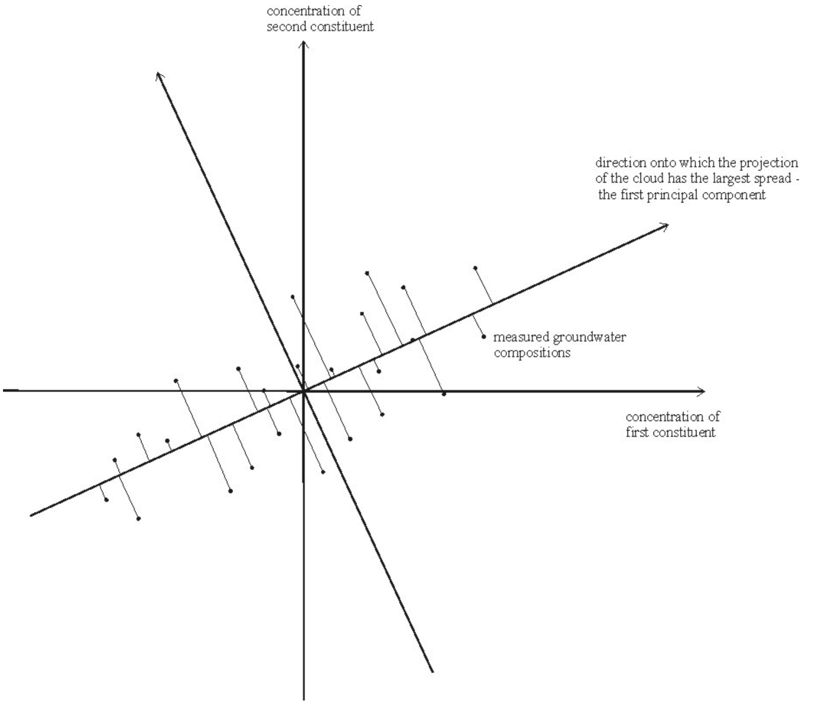


Figure 2-1 *Illustration of the process of determination of principal components, for a two-dimensional example.*

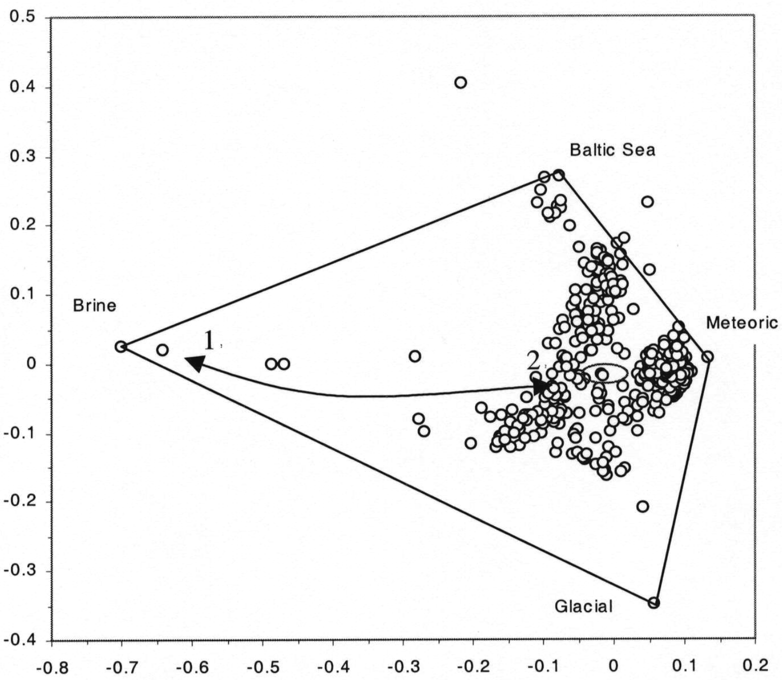


Figure 2-2 *The M3 plot for the groundwaters at Äspö that underlay most of the work done for Task 5.*

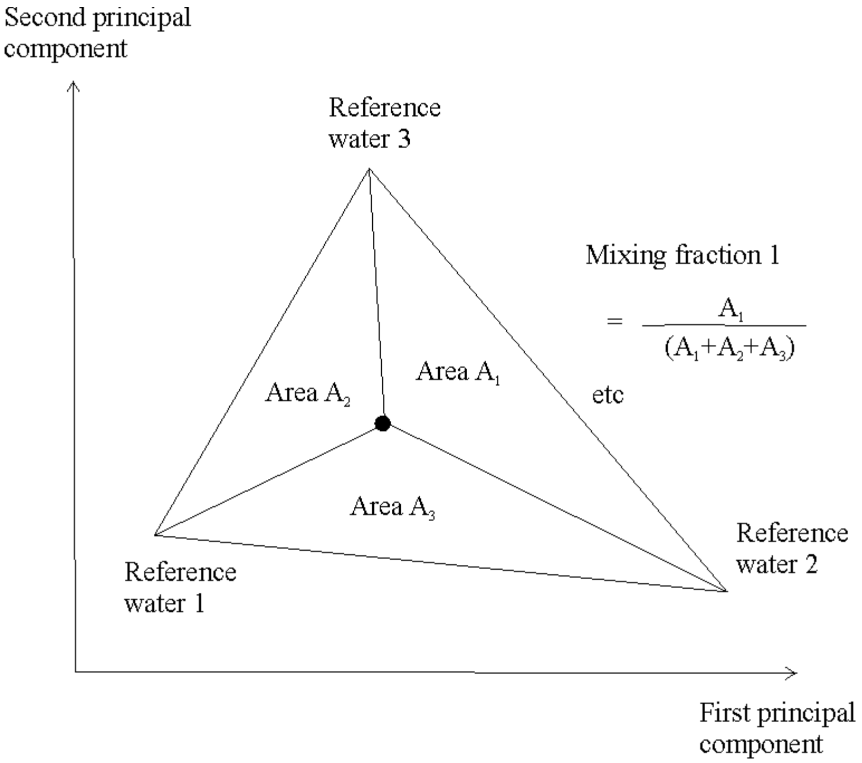


Figure 2-3 *The calculation of the mixing fractions for a case in which there are three reference waters.*

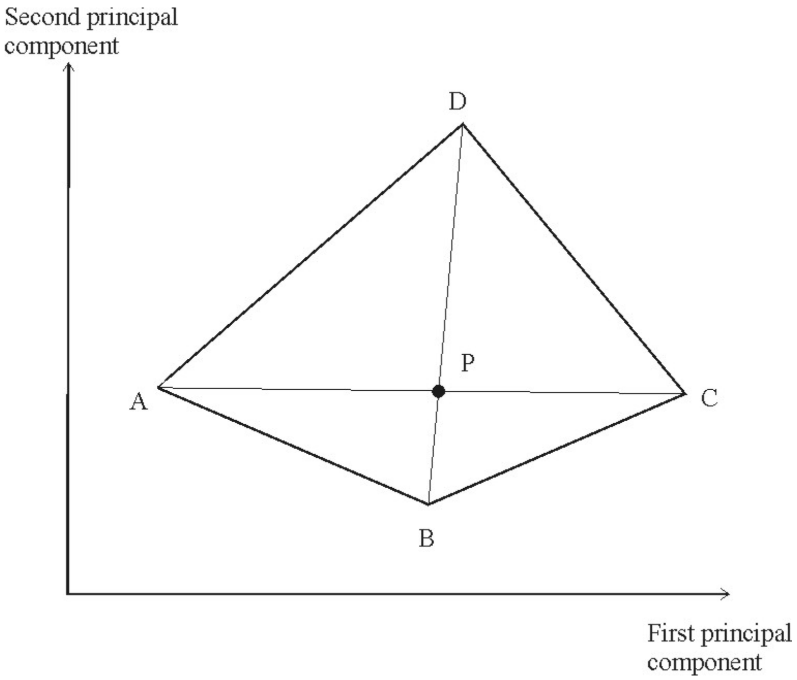


Figure 2-4 *Illustration of some of the potential ambiguity in the mixing fractions in a case in which there are more than three reference waters. (A sample with a composition corresponding to point P could be expressed as a mixture of reference waters A and C, or a mixture of reference waters B and D or a mixture of all four reference waters.)*

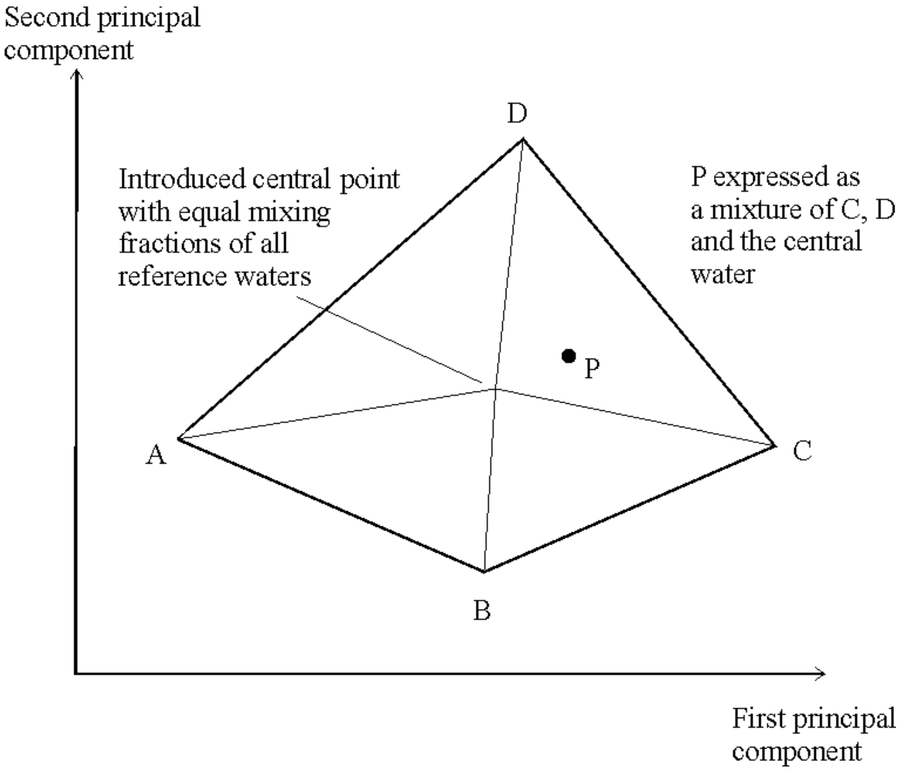
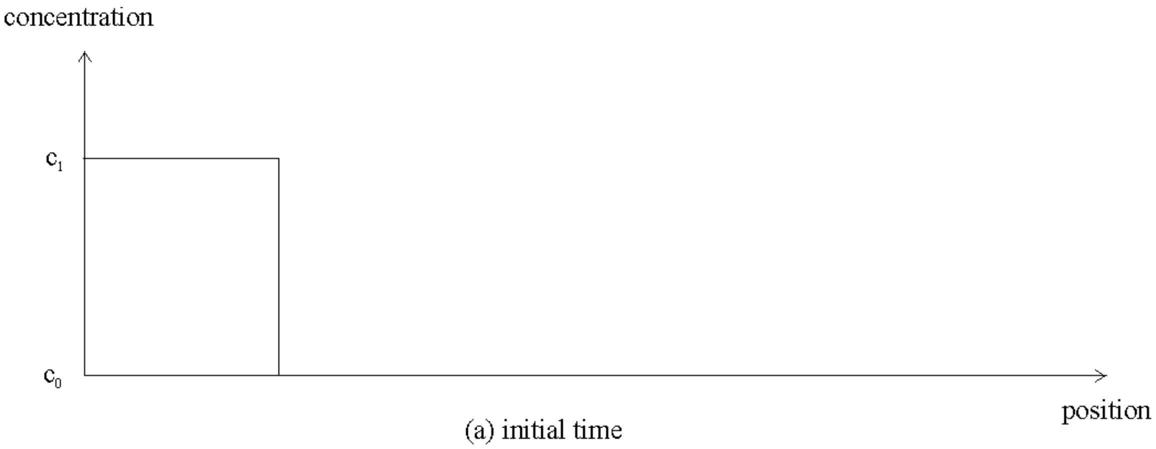
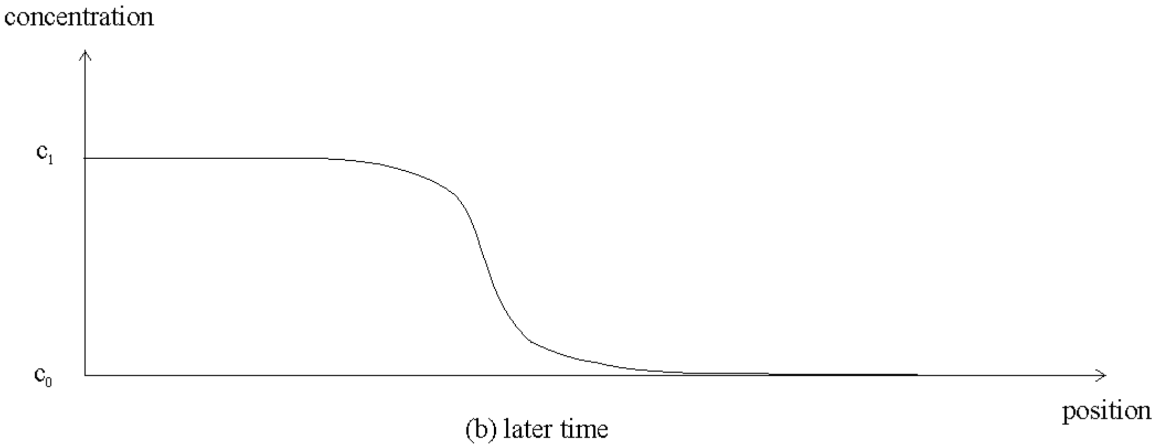


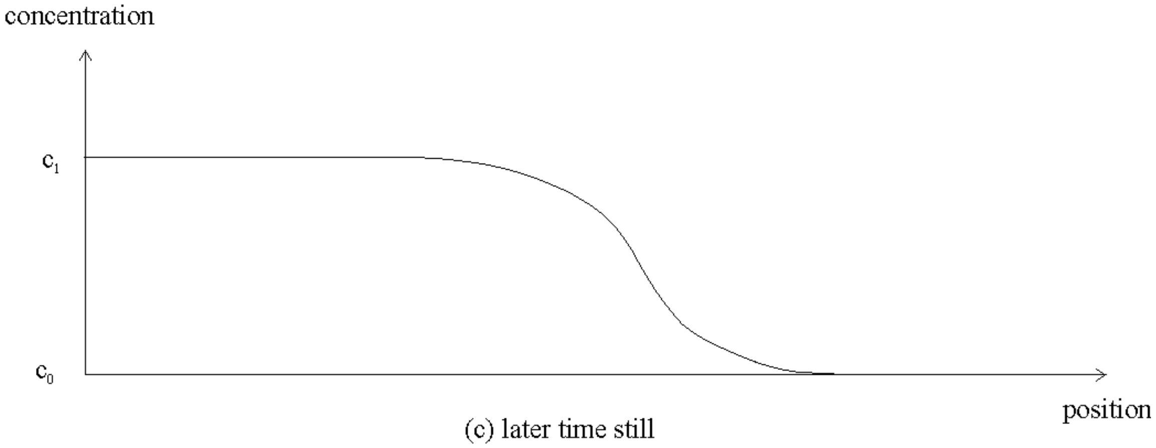
Figure 2-5 *Illustration of the approach used to remove the ambiguity in the M3 mixing fractions.*



(a) initial time



(b) later time



(c) later time still

Figure 2-6 *Evolution of the one-dimensional mixing zone corresponding to the analytic solution to the standard ADE given in Equation (16).*

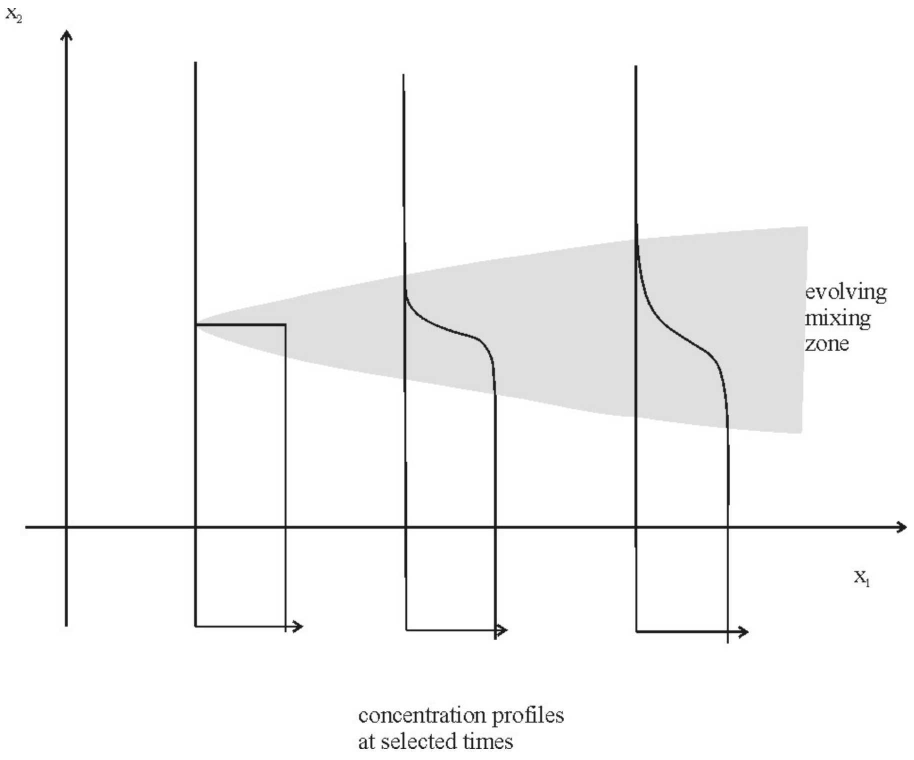


__Figure 2-7__ A two-dimensional mixing zone that is approximated by Equation (16).

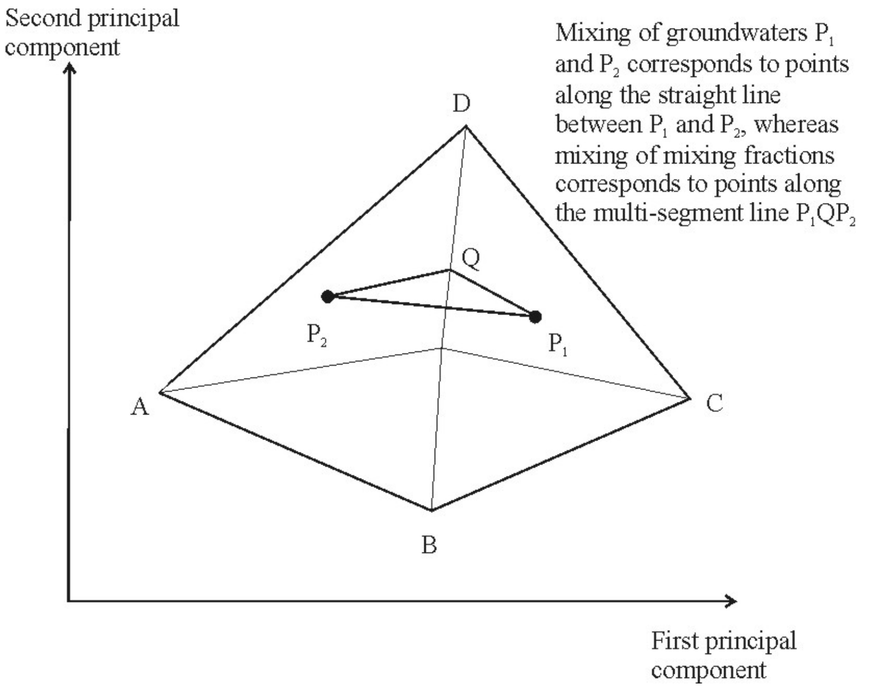


__Figure 2-8__ The mixing of different groundwaters.

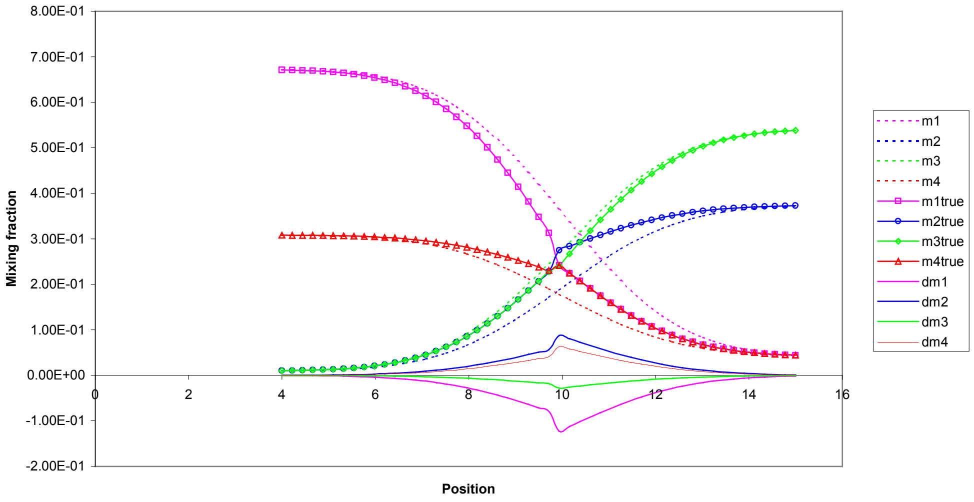


Figure 2-9 *An example of the comparison of mixing fractions calculated on the basis of the assumption that they obey the standard ADE with mixing fractions calculated from the equation that they really obey. (The dashed lines correspond to the mixing fractions calculated on the basis that they obey the standard ADE, the solid lines with symbols correspond to the mixing fractions calculated from the equations they really obey, and the solid lines give the errors.)*

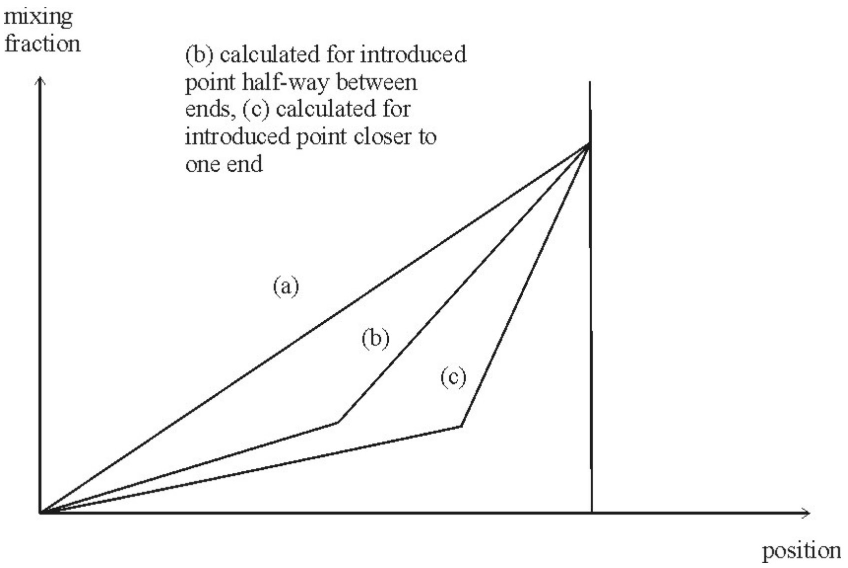


Figure 2-10 *Illustration of the reason for discrepancies greater than 0.25 between the mixing fractions calculated on the assumption that they obey the standard ADE and mixing fractions calculated from the equations that they really satisfy. The Figure shows the variation of one of the mixing fractions along a diagonal of the M3 polygon, in a case in which three of the reference waters have similar values for the first principal component, which lies along this diagonal, so that the central point in the M3 polygon is not in the middle of the line. (a) linear mixing between the end points. (b) the result of mixing if the central point is midway between the ends of the line; (c) mixing in the case in which the central point is not in the middle of the line.*

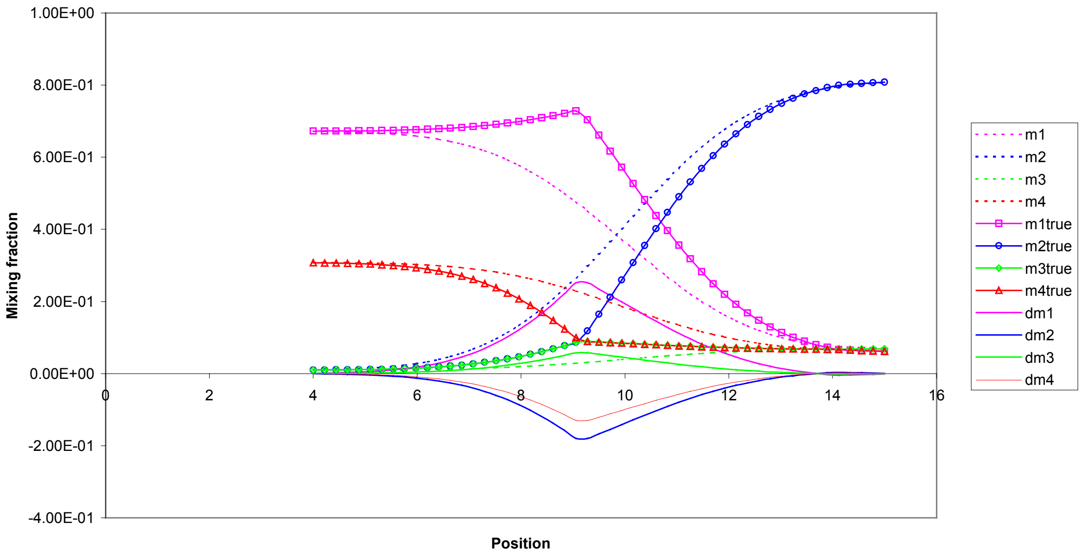


Figure 2-11 *Comparison of the mixing fractions calculated on the basis that they obey the standard ADE with mixing fractions calculated from the equations that they really satisfy, for a case in which one of the mixing fractions (the first) has an incorrect initial direction of change over the mixing zone. (The dashed lines correspond to the mixing fractions calculated on the basis that they obey the standard ADE, the solid lines with symbols correspond to the mixing fractions calculated from the equations they really obey, and the solid lines give the errors.)*

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