Technical Report

TR-05-14

Äspö Task Force on modelling of groundwater flow and transport of solutes

Review of Tasks 6A, 6B and 6B2

David Hodgkinson, Quintessa

John Black, In Situ Solutions

March 2005

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

Äspö Task Force on modelling of groundwater flow and transport of solutes

Review of Tasks 6A, 6B and 6B2

David Hodgkinson, Quintessa

John Black, In Situ Solutions

March 2005

Keywords: Review of Task 6A, Task 6B and Task 6B2, Tracer tests, Äspö Task Force, Modelling, Groundwater Flow, Transport of Solutes, Site characterisation, Performance assessment.

Abstract

This report forms part of an independent review of the specifications, execution and results of Task 6 of the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes, which is seeking to provide a bridge between site characterization and performance assessment approaches to solute transport in fractured rock.

The present report is concerned solely with Tasks 6A, 6B and 6B2 which relate to the transport of tracers on a 5-metre scale in Feature A at the TRUE-1 site.

The task objectives, specifications and individual modelling team results are summarised and reviewed, and an evaluation of the overall exercise is presented. The report concludes with assessments of what has been learnt, the implications for the Task 6 objectives, and some possible future directions.

Sammanfattning

Denna rapport utgör en del av en oberoende granskning av specifikationerna, utförandet och resultaten från Task 6 av ”Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes”. Task 6 syftar till att bygga en bro mellan ansatser rörande platsundersökningar och säkerhets- och funktionsanalys för transport av lösta ämnen i sprickigt berg.

Den aktuella rapporten behandlar endast Task 6A, 6B och 6B2, vilka i sin tur beskriver transporten av radioaktiva spårämnen på en 5 meters skala i ”Feature A” vid TRUE-1.

Syften, specifikationer och resultat från individuella modelleringsteam har sammanfattats och granskats och en utvärdering av den totala övningen har presenterats. Rapporten avslutas med en utvärdering av vilken kunskap som har kommit fram och vilka implikationer arbetet har för målen med Task 6 samt hur detta kan påverka inriktningen av framtida arbeten.

Executive summary

This report forms part of an independent review of the specifications, execution and results of Task 6 of the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes, which is seeking to provide a bridge between site characterization (SC) and performance assessment (PA) approaches to solute transport in fractured rock.

The present report is concerned solely with Tasks 6A, 6B and 6B2 which relate to the transport of tracers on a 5-metre scale in Feature A at the TRUE-1 site. The task objectives, specifications and modelling team results are summarised and reviewed. Also, an overall evaluation and review of the exercise is presented.

Task 6 is based on a extensive and well documented hydraulic and tracer data supported by extensive laboratory data. It addresses the important and challenging issue of how to bridge the gap between SC and PA modelling. The Äspö Task Force provides an excellent forum for addressing these challenges by bringing together the integrated expertise of experienced experimentalists and mathematical modellers within an international collaborative project.

Lessons learnt from this exercise, an assessment of the degree to which the Task 6 objectives have been addressed and achieved, and recommendations for the future are summarised below.

What have we learnt?

Flow

The quantitative description of water flow within and around Feature A still needs further refinement from the perspective of building confidence in a repository safety case, although it is likely to be adequate for performance assessment studies. This is reflected in the fact that most teams modelled Feature A as a single planar fracture despite some qualitative evidence to the contrary. Some teams accounted for channelling within the fracture plane due to transmissivity variability, but there is currently insufficient data to support such models.

Only one team attempted to model the small-scale three-dimensional hydraulic substructure of Feature A explicitly. This approach could provide a useful testing ground for understanding flow in complex fractures. For example, it is possible that where features consist of pseudo-parallel fractures, flow tends to jump between them and so is generally only in one fracture at a time.

For the other approaches the gap in understanding of the flow field on a millimetre and centimetre scale was essentially bridged by modelling assumptions. For example, a phenomenological flow aperture and a phenomenological transport aperture are often defined, but their precise relationship remains an open issue. Also, the flow-wetted surface (FWS) concept is often used but it depends on the flow path of the specific system and so is not rigorously defined. FWS is essentially an engineering approach, for example of relevance to heat exchangers where the geometry is reasonably well specified. The complexity and unbounded nature of geological features makes it very difficult to relate FWS to fundamental properties of the rock mass. Small-scale flow-related information will eventually be needed to demonstrate understanding of the system, for example the proposed resin injection experiments and detailed flow logging are likely to throw light on these issues.

Also, only one team modelled the three-dimensional flow connectivity with fractures in the surrounding rock mass. While the relatively high transmissivity and the large experimental pressure gradient ensured that most of the flow in the tracer test was along the one or two fault planes in Feature A, this will not necessarily be the case under natural long-term conditions.

In principle, tracer dilution data could be used as a further constraint on modelling the flow system. However, in practice this involves essentially arbitrary decisions about contributions from other pathways.

With the current state of knowledge, it is important to keep an open mind about the conceptualisation of flow in low permeability sparsely fractured rock. There are indications that flow may take place in relatively few discrete channels, rather than flow spread over the planes of fractures that are reasonably well connected.

An impressive range of conceptual and mathematical flow models was used in the study. In general all teams were able to calibrate their different models to the water travel time and dispersion for non-sorbed tracers. This demonstrates that the hydraulic data is not yet sufficient to discriminate between the different conceptual models.

However, it can be argued that Tasks 6A, 6B and 6B2 were primarily focussed on pore space interactions, with the flow field essentially specified, and thus it was not appropriate to direct too much effort towards the flow field.

Pore space interactions

A major achievement of the work reviewed here is the development of a consensus about the general conceptual model for diffusion and sorption of tracers into a range of pore spaces with different transport characteristics.

The modelling teams used a number of implementations of this conceptual model, and various methodologies were used to condition the models to the laboratory and field data. For example, Task 6 participants considered models with different immobile zones either parallel to or perpendicular to the main fracture. Both of these modelling approaches are clearly simplifications of a complex situation where different pore spaces with complex geometries are present at different places along the feature. There is clearly scope for developing further representations that capture the essence of the process interactions and are not unnecessarily complex. Nevertheless there was general agreement that short-term tracer tests only constrain the parameters of the most accessible pore spaces. Conversely, the rock matrix properties required for long-term performance assessments are not significantly constrained by such tests and need to be measured independently.

There is considerable documented geological evidence for the occurrence of pore space diffusion in the TRUE-1 block and at other locations, which provides a sound basis for the inclusion of this process by the modelling teams. Also, many analyses have deduced the action of matrix diffusion based on inverse power law tailing of tracer breakthrough curves. However, large effective values of diffusivity derived from such tailing can under some circumstances be due to hydrodynamic dispersion arising from tracer advection between slow and fast channels. Thus it would have been useful to have documented the reasons for assuming that the primary mechanism under the conditions of Tasks 6A, 6B and 6B2 is diffusion rather than dispersion.

Knowledge of the value of the β parameter is a major uncertainty in the modelling of tracer tests and in regard to extrapolating tracer migration to PA time scales. In particular it appears that this uncertainty is a major contributor to the wide range of results calculated by the different modelling teams. Moreover, there is currently little understanding of how the β parameter might vary between experimental and PA time scales.

With hindsight it would have been useful if more quantitative information about the immobile zones had been available. This would have narrowed the range of implementations of the basic conceptual model.

All of the groups assumed that sorption can be adequately modelled by a K_d factor representing linear equilibrium reversible process. While this may be a reasonable assumption for PA calculations, on experimental timescales kinetic effects may be important. Also, it can be argued that the K_d approach is a way of describing sorption rather than explaining it. Thus it is appropriate to continue to pursue research into more fundamental approaches to modelling chemical retention processes.

Tracer testing

As tracer tests only measure short-term behaviour, in future site characterization studies they should perhaps be used primarily with conservative tracers to establish connectivity, water travel time and dispersivity, rather than to study radionuclide transport processes.

However, tests using sorbing tracers have proved useful in demonstrating that it is not appropriate to use laboratory K_d values to interpret field tracer experiments, and that using laboratory values does not over-estimate sorption. Also, they have been important in understanding behaviour in and near fractures. Thus there is a case for continuing to carry out some tracer tests with sorbing tracers.

The radially-converging test configuration has proved valuable because there is a good possibility that all of the tracer will be recovered during the experiment, thereby reducing the ambiguity of the interpretation. It would be helpful in reducing the degrees of freedom of the interpretation if experiments could be carried out with more than one flow rate. However, in practice it has proved difficult to carry out experiments with significantly different flow rates. A key problem with tracer tests is the need to overcome the background flow. Thus it would be best to perform them where background flows are small, for example away from the immediate vicinity of drifts or using boreholes drilled from the surface.

It would also be useful to carry out tracer tests in less transmissive fractures that are more representative of the averagely fractured rock, and it is noted that some tests of this type are currently being performed as part of the TRUE Block Scale continuation programme.

Inverse modelling methodology

The probabilistic approach of the ANDRA-Golder team was successful in investigating a large section of parameter space and for propagating parameter correlations to performance assessment. It would have been interesting to have performed a cluster analysis of the selected solutions to see if they fell into reasonably well-defined conceptual model classes. Also, as demonstrated by the JNC-Golder team, it is useful to constrain theoretically-motivated parameter groups rather than individual parameters.

Forward transport modelling

While most groups assumed a single fracture geometry, with or without stochastic variability, based on the quantitative data in the specification, the JNC-LBNL group successfully incorporated qualitative geological structure information on the complexity of features, thereby enhancing the realism of the conceptual model. However, for PA modelling a valid approach is to use a simple fracture geometry but to include in the supporting description of the state of knowledge information on the complexity of features and how this may be represented appropriately in the PA representation using effective parameters. In this context, it is noted that Task 6 is providing important arguments for safety cases, primarily in the area of retention in immobile zones.

Forming a bridge between SC and PA modelling

Tasks 6A, 6B and 6B2 have been a useful learning exercise relating to the process of forming a bridge between SC and PA modelling. They illustrate that while laboratory and field characterisation data and associated SC modelling is necessary, it is rarely sufficient for PA. The key reason for this is that site characterisation can only quantify relatively short-term phenomena. Information or assumptions about long-term processes, for example from natural analogues, is also required.

The bridge building process is very important. We need to prove understanding, demonstrate that it is viable, check its consistency and subject it to independent review.

One problem with relatively complex SC models is that it is difficult to present the arguments clearly. Thus there will always be a need for simple bounding calculations.

In addition to the use of simplified PA models, there is a need to improve understanding of some processes and concepts in order to improve the level of confidence within the scientific community. In particular, the relationship of the β parameter, transport aperture and K_d to more fundamental structures and processes requires further study.

International modelling projects

The international collaboration dimension of the Task Force has been a key element in its success. It has provided a useful forum for the exchange of ideas among a peer group from similar organisations in different countries. For example this has led to an improved understanding of immobile zone interactions and has raised and discussed unresolved issues such as the β parameter. The Task Force also provides a useful training ground for researchers new to the field.

Over the past 15–20 years there have been significant advances in this field, and the Task Force has contributed significantly to these. However, care needs to be taken to ensure that the Task Force does not form a consensus that is blind to other perspectives. The commissioning of independent reviews, such as the present report, helps to guard against this possibility.

There is a need to communicate the work of the Task Force to the scientific community, and thus it would be beneficial if there were more presentations of Task Force work at conferences, and papers published in peer-reviewed journals.

The manner in which the Task Force is conducted is an important ingredient of its success. The Task Force is a very civilised forum where due respect is given to alternative views. Sometimes this can manifest itself as a lack of discussion and argument following presentations. However, the meetings clearly have an impact on the work of the modelling groups, for example in modifications to approaches presented at subsequent meetings.

The exercise reviewed here can be viewed as a form of integrated conceptual model sensitivity study of the residual uncertainty remaining after the system has been constrained by tracer test data and other site characterisation information. One disadvantage of such an exercise being carried out as part of an international project is that the modelling teams act rather independently of each other. For the future it might be worthwhile to consider stronger coordination, for example a task leader or core group who could steer the exercise on a more frequent basis than was possible at the Task Force meetings.

What are the implications for the Task 6 objectives?

The first objective of Task 6 is to assess the simplifications used in PA models. Key assumptions for long-term PA predictions are the general characteristics of the water flow paths and the extent to which dissolved radionuclides can diffuse and sorb within the rock matrix. If it is assumed that flow from a repository only occurs along a network of paths similar to the fault plane(s) within Feature A then this could considerably underestimate the degree of interaction of radionuclides with the rock mass. This may be reasonable if a pessimistic philosophy is adopted in the PA, but increasingly PAs and associated safety cases are tending to adopt more realistic approaches. If a more realistic approach is to be adopted then account needs to be taken of the hydraulic sub-structure of features such as Feature A, and connectivity with fractures in the surrounding rock mass.

As demonstrated by the results of the modelling teams, a key assumption is to distinguish between the diffusion parameters derived from short-term tracer tests and those required for PA. In particular, a number of teams have demonstrated that a suitable PA representation is to incorporate all the rapid near-fracture processes into an effective surface retardation coefficient, and diffusion into the intact rock via a one-dimensional diffusion/sorption equation.

The methodologies used by the modelling teams included deterministic best fits of model parameters to test data, with and without sensitivity analysis, and probabilistic sensitivity analysis. Some form of sensitivity analysis is appropriate for providing input to PA in order to propagate appropriate uncertainties. However, if parameters are represented by uncorrelated distributions, when in reality they should be correlated, then the overall PA uncertainty would be over-estimated. A practical solution to this problem has been advocated by the ANDRA-Golder team in terms of a probabilistic sensitivity analysis methodology that propagates vectors of parameter combinations, that are consistent with experiments, to PA. Also, correlations can be accounted for in terms of theoretically-motivated parameter groups and in this context it is interesting that the JNC-Golder team found that for Task 6A the physical parameters of the solute transport model were not well constrained, but parameter groups such as the mobile/immobile volume ratio were constrained.

The second objective of Task 6 is to determine how, and to what extent, experimental tracer and flow experiments can constrain the range of parameters used in PA models. Short-term tracer tests are generally performed in high transmissivity features, which are not necessarily representative of the rock mass as a whole. Thus the results from such experiments do not constrain the range of fracture flow parameters required for PA unless a pessimistic PA approach is adopted. For pore space interactions it has been demonstrated by the modelling teams that short-term tracer tests do not constrain the parameters to be used for PA. These conclusions have been effectively quantified using probabilistic assessments of the degree to which the tracer tests constrain prior model parameter distributions and output distributions for subsequent PA calculations.

The third objective of Task 6 is to support the design of site characterisation programmes to assure that the results have optimal value for performance assessment calculations. It is concluded that site characterisation programmes should include direct measurements of the diffusion and sorption parameters for the intact rock matrix. The β parameter has been shown to be critical for understanding the transport of solutes in fractured rock. However, at present it is poorly characterised and definitions vary between implementations. New ways need to be found to derive reliable estimates of this parameter under SC conditions, for example by using resin injection and detailed flow logging.

The fourth objective of Task 6 is to improve the understanding of site-specific flow and transport behaviour at different scales using site characterisation models. There is a need to develop a more realistic understanding of the flow paths within and around features such as Feature A by combined experimentation and modelling. Tasks 6A, 6B and 6B2 have taken a useful step along this path, but the lack of discrimination among very different flow geometries demonstrates that more work is required in this area.

Where do we go from here?

The foundation of all solute transport modelling is a sound understanding of the characteristics of the flow paths. Even for a feature of the limited size of Feature A, which has been extensively characterised, there remain many open questions as to the flow geometry and characteristics. It is thus recommended that flow within the sub-features that constitute Feature A, or similar features, is investigated in greater detail both experimentally and through more detailed modelling studies to throw greater light on the characteristics and effects of phenomena such as flow channelling, multiple near-parallel fractures, and the β parameter.

Feature A lies at the high end of the spectrum as regards transmissivity and connectivity at Äspö. Accordingly it is recommended that similar studies are made of features in the middle of the spectrum, in the so-called averagely fractured rock.

The connectivity of the rock mass as a whole is also of relevance. There are indications of compartmentalisation of flows at Äspö and at other low permeability crystalline rock sites, which might usefully be addressed in future by the Äspö Task Force.

The present exercise has improved the state of knowledge of how advecting tracers interact with stagnant pore spaces. However, the analysis of diffusion and sorption in these pore spaces is complicated by the fact that the water is moving rapidly in channels of unknown geometry and with poorly characterised β parameter. To probe diffusive transfer and chemical interactions in the rock matrix more deeply it would be advantageous to separate flow from diffusive transport by analysing experiments in which stationary tracer solutions are kept in contact with fracture surfaces of known area. Moreover, such experiments could also be used to make a more in-depth analysis of the chemical interactions between solutes and rock, making use of reactive geochemical transport codes. In order to address long-term issues it would also be useful to apply such models to the analysis of natural analogue data for near-fracture chemical alteration.

Contents

1 Introduction and objectives

1.1 Background

Safety cases for the geological disposal of radioactive waste require a sound understanding of potential scenarios in which radionuclides are leached from damaged or degraded canisters and are transported in groundwater through the surrounding rock mass.

For crystalline rock, water flows predominantly through channels within interconnecting fractures /Abelin et al. 1985, 1990; Bourke, 1987; Moreno and Neretnieks, 1993/ and solutes are retarded by diffusion into non-flowing water in the fractures and rock, and by chemical interactions with the rock. A detailed understanding of these processes requires the integrated expertise of experimentalists and mathematical modellers and benefits from international collaboration. These three strands have been woven together within the Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes /SKB, 2003/, building on earlier work within the International Stripa Project /NEA and SKB, 1994/.

1.2 Äspö Hard Rock Laboratory

The Äspö Hard Rock Laboratory (HRL) /SKB, 2003/ is situated on the east coast of Sweden (Figure 1-1) and provides facilities for research, development and demonstration in relatively undisturbed crystalline rock down to anticipated repository depths (Figure 1-2).

Figure 1-1. Location of the Äspö Hard Rock Laboratory /Winberg et al. 2000/.

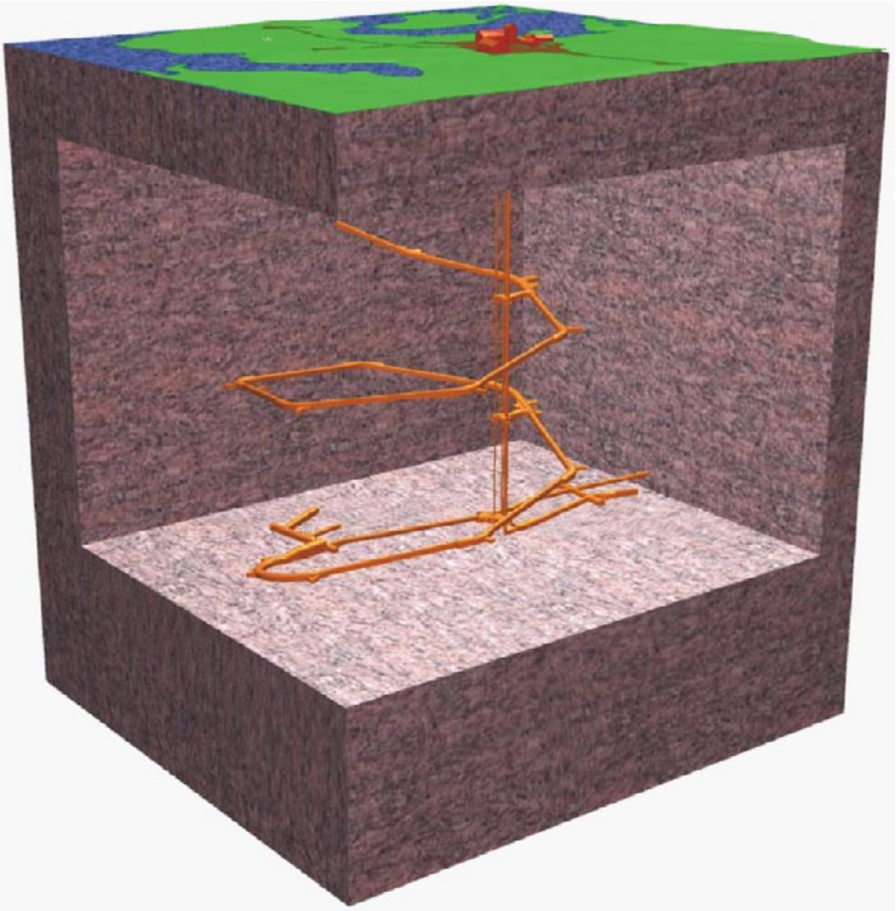

Figure 1-2. Outline of the Äspö Hard Rock Laboratory /Winberg et al. 2000/.

1.3 TRUE Programme

The overall objectives of the Tracer Retention Understanding Experiments (TRUE) programme /Bäckblom and Olsson, 1994/ are to:

- develop the understanding of radionuclide migration and retention in fractured rock;
- evaluate to what extent concepts used in models are based on realistic descriptions of fractured rock and if adequate data can be collected in site characterisation programmes;
- evaluate the usefulness and feasibility of different approaches to modelling radionuclide migration and retention; and
- provide in situ data on radionuclide migration and retention.

A staged approach has been adopted to address these ambitious objectives. This review relates to work performed during the first stage (TRUE-1) that was concerned with flow and transport on a detailed (0.5–10 m) scale with the specific objectives /Winberg, 1994; Winberg et al. 2000/ to:

- conceptualise and parameterise an experimental site using tracer tests with conservative and sorbing tracers in a simple test geometry;
- improve methodologies for conservative tracer tests; and
- develop and test a technology for injection of epoxy resin and techniques for excavation of injected volumes and subsequent analysis.

The TRUE-1 experimental site (Figure 1-3) is bounded by a group of site-scale fracture zones (NW-2, NNW-4, NW-3). Conductive features within the TRUE-1 site were identified and correlated between five boreholes from inflows during drilling and associated pressure responses, detailed single packer flow logging, and cross-hole interference tests /Winberg et al. 2000/.

The present review relates to tracer transport within Feature A, which is a near-planar feature that intersects all five boreholes (Figure 1-4). A schematic conceptual realisation of Feature A is shown in Figure 1-5 /Winberg et al. 2000/.

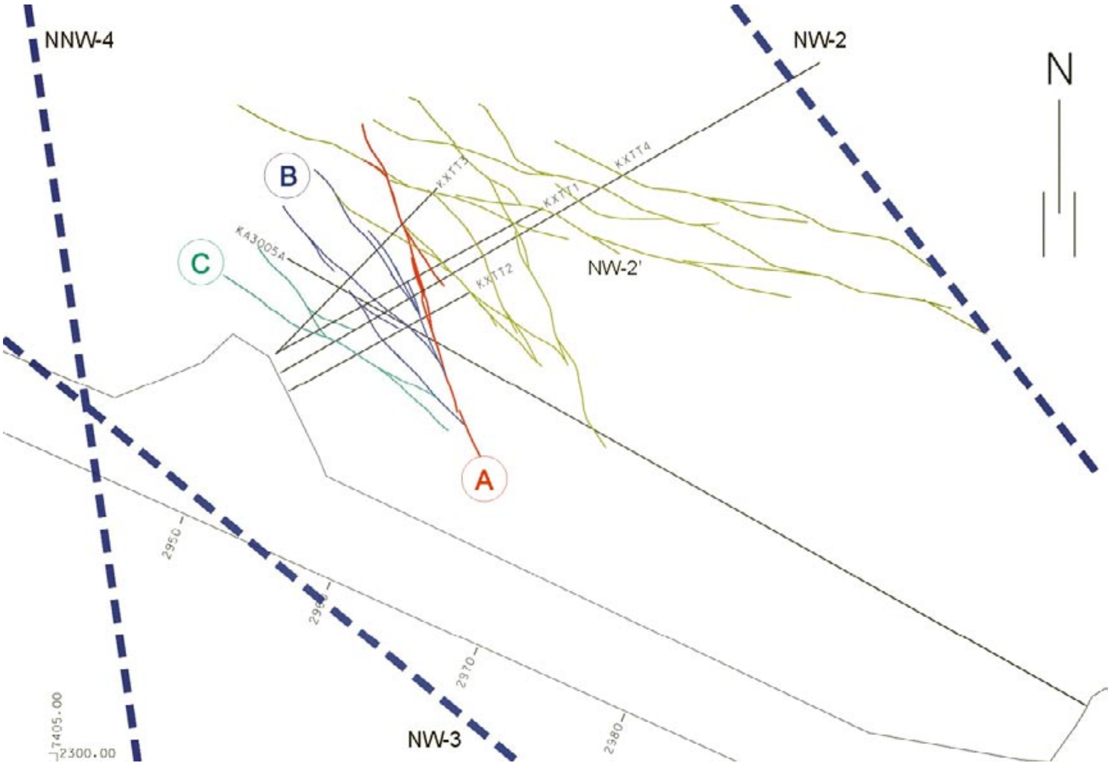

Figure 1-3. *Horizontal section at 400 m below sea level showing the identified conductive geological structures at the TRUE-1 site /Winberg et al. 2000/.*

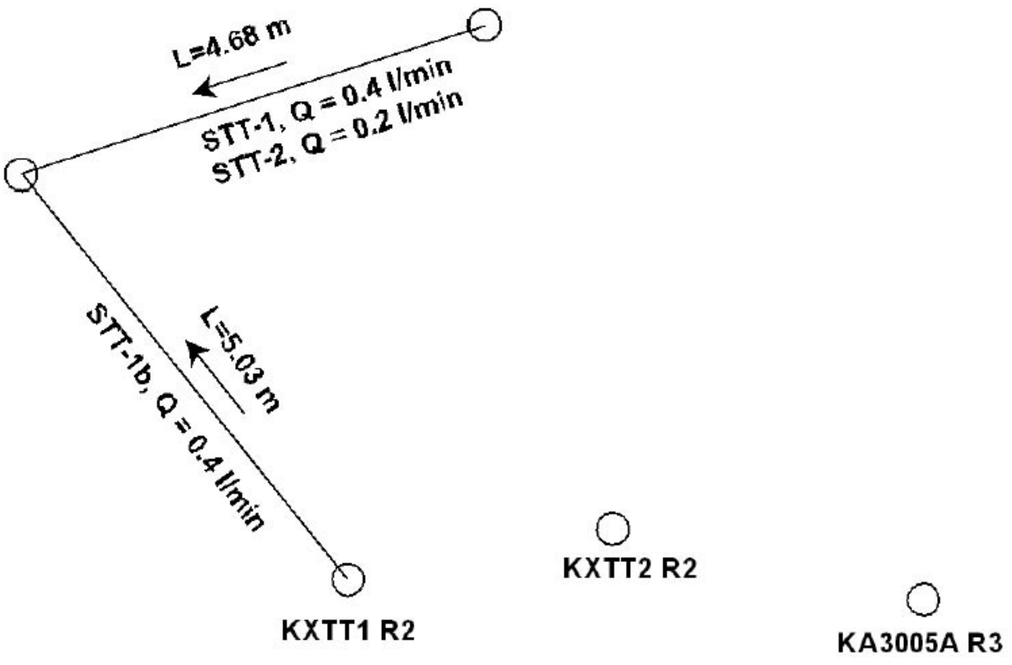

Figure 1-4. Intersection of Feature A with the five boreholes together with the geometry and pumping flow rates (Q) the tracer tests STT-1, STT-1b and STT-2 /Selroos and Elert, 2001/.

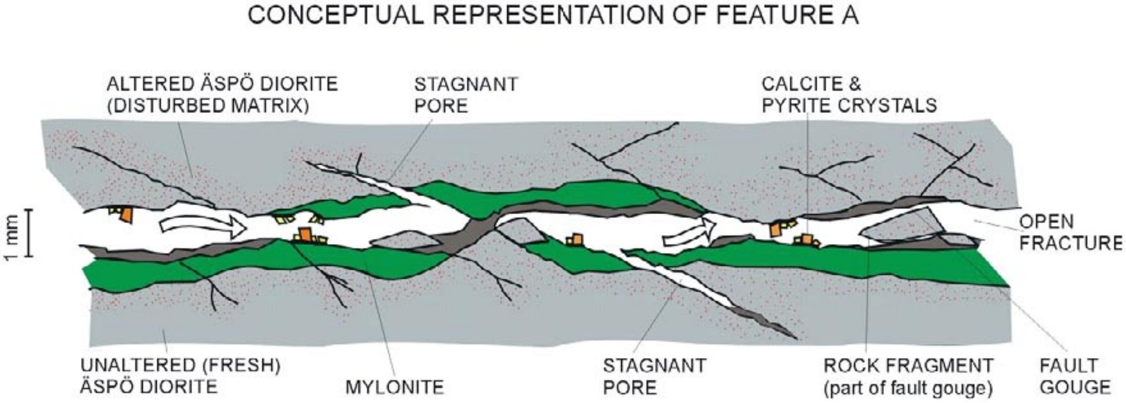

Figure 1-5. Schematic conceptual cross-section (not to scale) of Feature A /Selroos and Elert, 2001/.

1.4 Äspö Task Force

The Äspö Task Force (TF) on Modelling of Groundwater Flow and Transport of Solutes was set up in 1992 as a forum for international cooperation. Each participating organisation is invited to form or appoint a team to carry out parallel modelling of Äspö HRL experiments.

The work is performed within the framework of well-defined and focused modelling tasks. The TF endeavours to evaluate different concepts and modelling approaches. This is achieved by several modelling teams performing the same task followed by evaluation of the modelling work by the TF delegates. The modelling efforts of the Task Force provide information on how different model concepts can be applied in fractured rock and, in particular, allow identification of important parameters needed to perform predictive modelling of radionuclide transport.

To date the following five Tasks have been completed and reported.

Task 1: Pumping, tracer and dilution tests on a site scale (1 km) /Gustafson and Ström, 1995/.

Task 2: Design calculations for a number of planned field tracer experiments at the Äspö site on a detailed scale (1–10 m) /Selroos et al. 1994/.

Task 3: The hydraulic impact of the Äspö tunnel excavation at site scale (1 km) /Gustafson et al. 1997/.

Task 4: Radially converging tracer tests and dipole tests on a detailed scale (1–10 m) /Marschall and Elert, 2003/.

Task 5: Integration of hydrogeology and hydrochemistry: a model assessment exercise focussed specifically on the impact of the HRL tunnel construction on the groundwater system at Äspö /Rhén and Smellie, 2003/.

1.5 Scope and objectives of Task 6

Task 6 seeks to provide a bridge between site characterization (SC) and performance assessment (PA) approaches to solute transport in fractured rock. This is addressed by considering two spatial scales (a single feature and a network scale) and two temporal scales (SC and PA time scales).

In Task 6 both PA and SC models are applied to tracer experiments considering both the experimental boundary conditions and boundary conditions of relevance to PA. The approach is firstly to implement models such that they can reproduce the results from relevant Äspö in situ tracer experiments. Appropriate assumptions for PA modelling are then made, while continuing to honour the in situ tracer experimental results.

There is no strict distinction between SC and PA models. However, in general SC models aim to reflect realistic geological complexity and are focussed on phenomena which vary over time scales of less than a year. In contrast, PA models generally adopt more conservative geometric assumptions and include slower processes in order to demonstrate with reasonable confidence that repository safety targets are not exceeded over periods in excess of thousands of years.

The objectives of Task 6 have been set out by /Benabderrahmane et al. 2000/ as follows.

1. To assess simplifications used in PA models including:
    a. identifying the key assumptions and the less important assumptions for long-term PA predictions;
    b. identifying the most significant PA model components of a site;
    c. prioritisation of PA modelling assumptions and demonstration of a rationale for simplification of PA models by parallel application of several PA models of varying degrees of simplification;
    d. provision of a benchmark for comparison of PA and SC models in terms of PA measures for radionuclide transport at PA temporal and spatial scales; and
    e. establishment of a methodology for transforming SC models using site characterisation data into PA models in a consistent manner.

2. To determine how, and to what extent, experimental tracer and flow experiments can constrain the range of parameters used in PA models.
3. To support the design of site characterisation programmes to assure that the results have optimal value for performance assessment calculations.
4. To improve the understanding of site-specific flow and transport behaviour at different scales using site characterisation models.

The scope of Task 6 covers seven sub-tasks as follows.

Task 6A models selected TRUE-1 tests in order to provide a common reference platform for all SC and PA modelling to be carried out in subsequent tasks, thereby ensuring a common basis for future comparison.

Task 6B models selected PA cases at the TRUE-1 site with PA relevant (long term/base case) boundary conditions and temporal scales. This task serves as a means to understand the differences between the use of SC and PA models, and the influence of various assumptions made for PA calculations for extrapolation in time.

Task 6B2 is similar to Task 6B except that the boundary conditions are modified to produce flow and transport over a larger area of Feature A. The input boundary is no longer a point source and the tracers are assumed to be collected in a fracture intersecting Feature A.-

Task 6C is concerned with the development of a 50–100 m block scale synthesised structural model with a hydraulic parameterisation. A deterministic rather than a stochastic model is used so that the differences between models result from variations in assumptions, simplifications and implementation rather than from the structural framework.

Task 6D is similar in purpose to Task 6A, but is based on the synthetic structural model developed in Task 6C and a 50 to 100 m scale TRUE-Block Scale tracer experiment. This task provides a common reference platform for all SC and PA modelling at the network scale and ensures a common basis for Task 6E.

Task 6E extends the Task 6D transport calculations to a reference set of PA time scales and boundary conditions. The first part of Task 6E uses a basic set of PA and SC assumptions and simplifications while in the second part a sensitivity analysis is carried out by investigating the effects of alternative assumptions.

Task 6F consists of a series of “benchmark” studies on single features from the Task 6C hydro-structural model in order to improve the understanding of differences between the participating models.

1.6 Scope and objectives of review

This report forms part of an independent review of the specifications, execution and results of Task 6. The review has been carried out by:

- reviewing background reports on the TRUE programme;
- reviewing the Task 6 specifications, modelling team reports and questionnaire responses;
- participating in Äspö Task Force workshops and meetings; and
- discussions with individual modelling teams.

The present report is concerned solely with Tasks 6A, 6B and 6B2. In order to produce a self-contained document, this report summarises pertinent aspects of the tasks. Also, an evaluation of the modelling team results is included. Thus in essence it is a summary, evaluation and review report.

Section 2 presents a summary of the task specifications followed by review comments on the specifications.

Following an overview of the work of the modelling teams, the sub-sections of Section 3 consider the work of each modelling team in turn. Their approaches and key results are summarised and discussed followed by review comments on the work of each team.

Section 4 presents an overall evaluation and review of the work of the entire exercise consisting of the work of all modelling teams for Tasks 6A, 6B and 6B2.

Finally, Section 5 presents the conclusions of this review, including lessons learnt, an assessment of the degree to which the Task 6 objectives have been addressed and achieved, and recommendations for the future.

2 Task specifications

The task specifications are summarised in Sections 2.1 to 2.4 and review comments on the specifications are presented in Section 2.5.

2.1 Input data

This section summarises the range of background information provided to the modelling teams in the Task 6A and 6B specification document /Selroos and Elert, 2001/ including information on possible alternative conceptual models.

2.1.1 Geometry of Feature A

Feature A is estimated to have an extent of about 10–20 m. No intercepts with the tunnel have been observed, and available hydraulic information support the fact that Feature A is not in hydraulic contact with the tunnel. A planar structure fitted through the five interpreted borehole intercepts has an orientation of N29W/79E. The borehole intercepts indicate one, or alternatively two, sub-parallel fault planes. The total thickness of the feature varies between 0.05 m and 0.09 m and the physical aperture of the fracture is assumed to be variable in the range of 1–3 mm.

2.1.2 Geological interpretation of Feature A

Feature A is believed to be a reactivated mylonite which has been exposed to subsequent brittle deformation forming the main fault plane, which in turn is believed to be the main conductive element of Feature A. Feature A essentially follows the mylonite, and is interpreted to be bounded by a rim zone consisting of altered Äspö diorite which constitutes a band of disturbed rock along the feature. The main difference between the two lithological units relates to the mineralogical composition, grain size and porosity.

The fault plane is not centred on the mylonite along its extent and thus water is assumed to be interchangeably in contact either with mylonite or with altered Äspö diorite. The main fracture minerals are calcite, fluorite, quartz, k-feldspar and pyrite, found as idiomorphic crystals. There is evidence of clay minerals as an outer rim of the fracture mineral coating, which suggests that gouge material may be present in Feature A. However, this has not been substantiated by cores intersecting Feature A, but later drilling using triple tube techniques shows hard evidence of fault gouge in structures similar to Feature A. It is assumed that the gouge material apart from a fine clay fraction consists of macro-sized fragments of primarily altered Äspö diorite.

2.1.3 Alternative conceptual models

In order to set the scene, the specification document provided information on the TRUE-1 conceptual model, discussed above, together with two alternative conceptual models, the FCC model and the KTH-ChE model, summarised below. However, it was emphasised that the modelling teams were free to use any conceptual model that they could motivate.

The FCC conceptual model of the TRUE-1 block is based on the results of the Fracture Characterization and Classification (FCC) project, which is documented in /Mazurek et al. 1997/ and /Bossart et al. 2001/. The FCC project aimed to develop an understanding of the present-day fracture network and its evolution over geological time including recurrent events of hydrothermal water/rock interaction.

The TRUE-1 volume is penetrated by a dense network of interconnected fractures of different orientations with the majority of all fractures being less than 1 m extent. Feature A is one of a minority of fractures with reactivated mylonitic precursors. It is considered unlikely that Feature A is one discrete structure. It is more likely a cluster of shorter, interconnected fractures that concentrate along the mylonitic precursor. Moreover, this fracture cluster is interconnected in three dimensions with fracture systems that are unrelated to the mylonitic precursor.

Rock units that occur in or adjacent to fractures may differ substantially from those of the bulk volume of the rock, which consists largely of unaltered granite. As shown in Figure 2-1 it is possible to distinguish fresh or altered granite, fresh or altered mylonite, cataclasite (cemented brittle fault rock) and fault gouge (uncemented, cohesionless brittle fault rock). The diffusion-accessible porosities of the fault rocks are substantially higher than those of granite and mylonite. Moreover, fault gouge and cataclasite contain clay minerals, including smectite layers, from which a much higher sorption capacity can be inferred. Thus it may be inferred that relatively small volumes of rock that have a retardation capacity much higher than granite occur along fractures.

In the cross-hole tracer experiments considered here the pumping rates were substantial, and the width of the flow field was in the range of centimetres /Jakob and Heer, 2000/ with the result that flow is largely one-dimensional. In contrast, the hydraulic gradients in a natural system are much smaller and thus flow could take place in more dimensions and over larger scales.

Consequently over the short experimental timescales of Task 6A, tracer retardation is likely to occur exclusively in the rock units immediately (mm-cm) adjacent to the fracture(s). The most likely candidates are fracture-filling fault gouge and adjacent cataclasite, because these rock units have the largest diffusion-accessible porosity and sorption capacity. No direct measurements are available for the sorption characteristics of these materials, and so they need to be inferred from inverse modelling of tracer tests or from the general scientific literature. For the longer timescales of Task 6B and 6B2, retardation will additionally be affected by the more intact rock further away from the fractures.

In contrast, the KTH-ChE model /Neretnieks and Moreno, 2000/ envisages Feature A as a cluster of interconnected fractures that can lead to flow in three dimensions with rock matrix diffusion and sorption properties representative of intact rock. This is discussed further in Section 3.11.

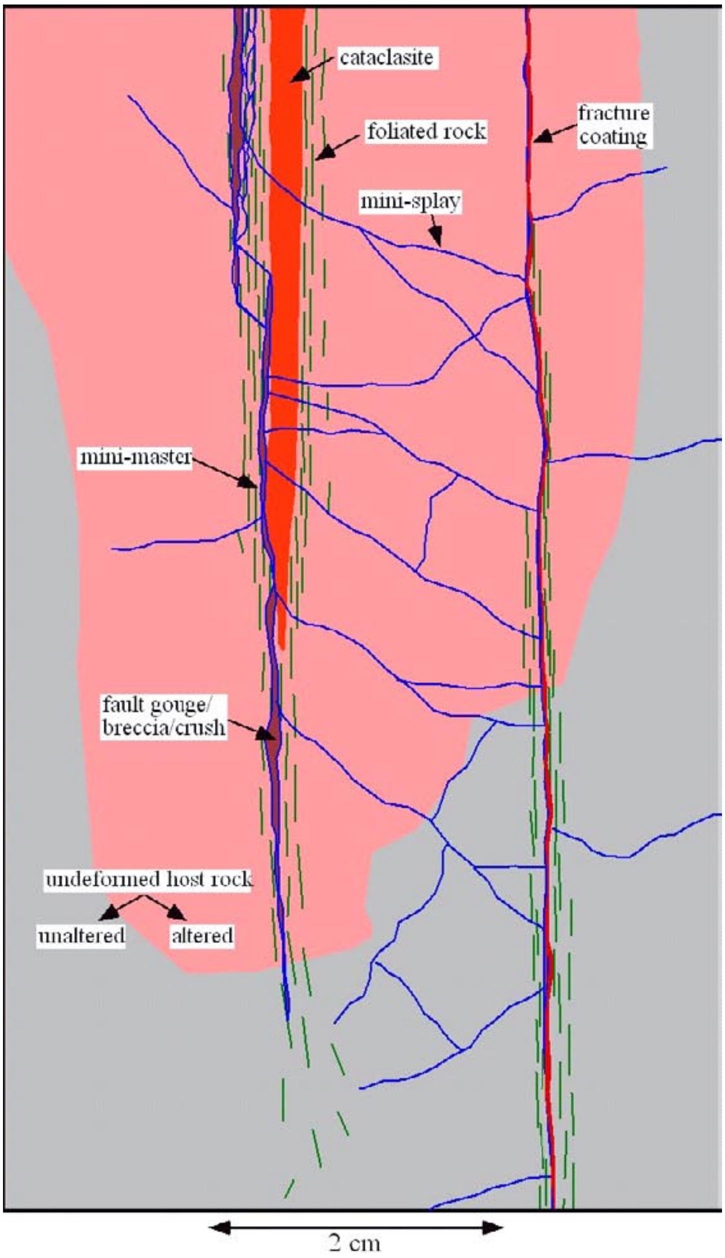

***Figure 2-1.** Small-scale anatomy of a master fault /Selroos and Elert, 2001/.*

2.1.4 Tracer test STT-1b

Tracer test STT-1b /Andersson et al. 1999/ was performed using a radially converging flow geometry with pumping in borehole section KXTT3 R2 and injection of tracer in borehole section KXTT1 R2, both penetrating Feature A (see Figure 1-4). The distance between the boreholes was 5.03 m.

The hydraulic heads (metres above sea level) in the sections containing Feature A prior to the STT-1b tracer test were KXTT1 R2 (–53.02), KXTT2 R2 (–53.03), KXTT3 R2 (–52.62), KXTT4 R3 (–52.88) and 3005A R3 (–53.57). The density of the water is estimated to be 1,005 kg/m^3.

The passive injection section (KXTT1 R2) was equipped with a circulation system where a solution containing twelve different tracers was injected as a finite pulse with a duration of 4 hours. Four non-sorbing (uranine, HTO, ^{82}Br, ^{131}I) and six weakly to moderately radioactive sorbing tracers (^{22}Na, ^{42}K, ^{85}Sr, ^{99m}Tc, ^{58}Co and ^{86}Rb) were used. After four hours of injection the tracer solution was exchanged in two steps with unlabelled water. The first exchange lasted for 60 minutes and the second exchange, following a delay of 100 minutes, lasted for 25 minutes. The injection concentration time histories (Bq/kg) for the STT-1b tracer test (Figure 2-2) were supplied to the modelling teams. The flow rate in the injection section was estimated to be 41.9 ml/h during the period 0–4 hours and 58.1 ml/h during the period 20–151 hours. Because of the flushing of the injection section no estimates could be made for the period 4–20 hours. The injection time histories of americium and technetium are assumed to be identical to that of cobalt. The pumping in the withdrawal section (KXTT3 R2) was 0.401 l/min.

Breakthrough curves from the STT-1b tracer test are available for ^{131}I, ^{85}Sr and ^{58}Co together with a number of other non-sorbing or weakly sorbing tracers (Figure 2-3). No recovery was observed for ^{99m}Tc, which is attributed to the fact that technetium is strongly sorbing under the expected reducing conditions. The measured breakthrough curves were deconvoluted to produce equivalent breakthrough curves for a Dirac delta function input in order to assist in the evaluation of modelling results /Elert and Svensson, 1999, 2001/.

For calibration purposes, the results of other hydraulic and tracer tests performed in Feature A within TRUE-1 were made available to the modelling teams.

Tracer test STT-1b was previously modelled in Task 4E. In that exercise the modelling teams were provided with site characterization data, together with data from preliminary tracer tests with non-sorbing tracers, and laboratory measurements of retention parameters (D_e, K_a and K_d). The objective was to predict tracer breakthrough based on the supplied information. The predictions for sorbing tracers using the laboratory measurements of retention parameters generally underestimated the breakthrough time. In order to have

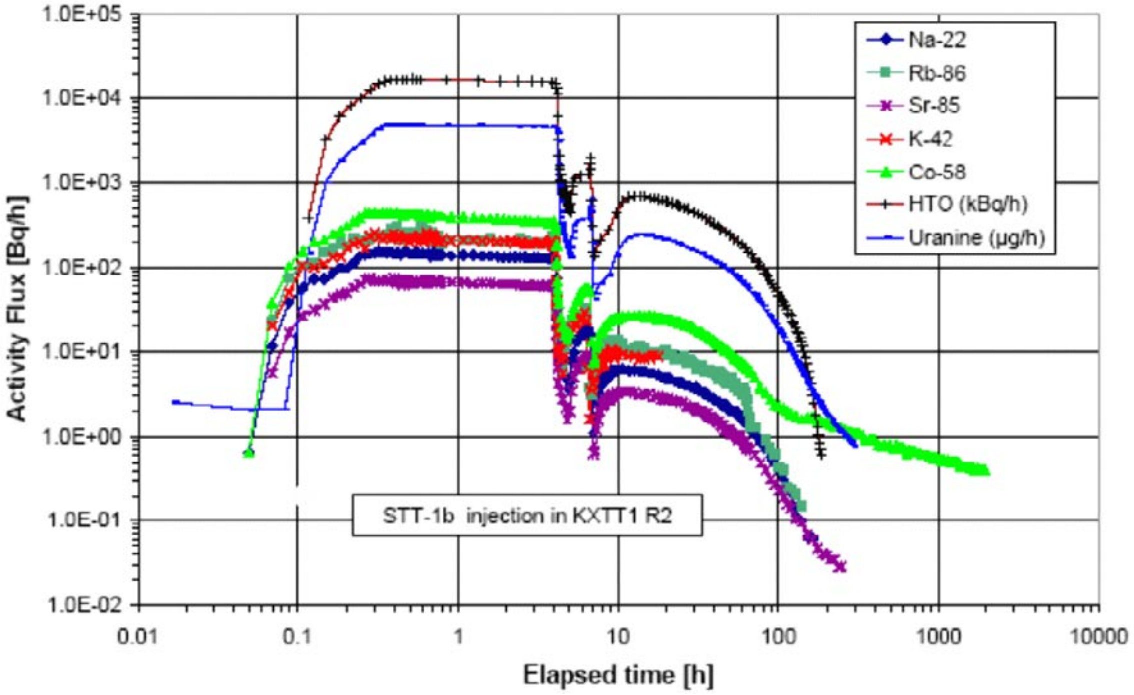

***Figure 2-2.** Injection flux of tracers in STT-1b /Andersson et al. 1999/.*

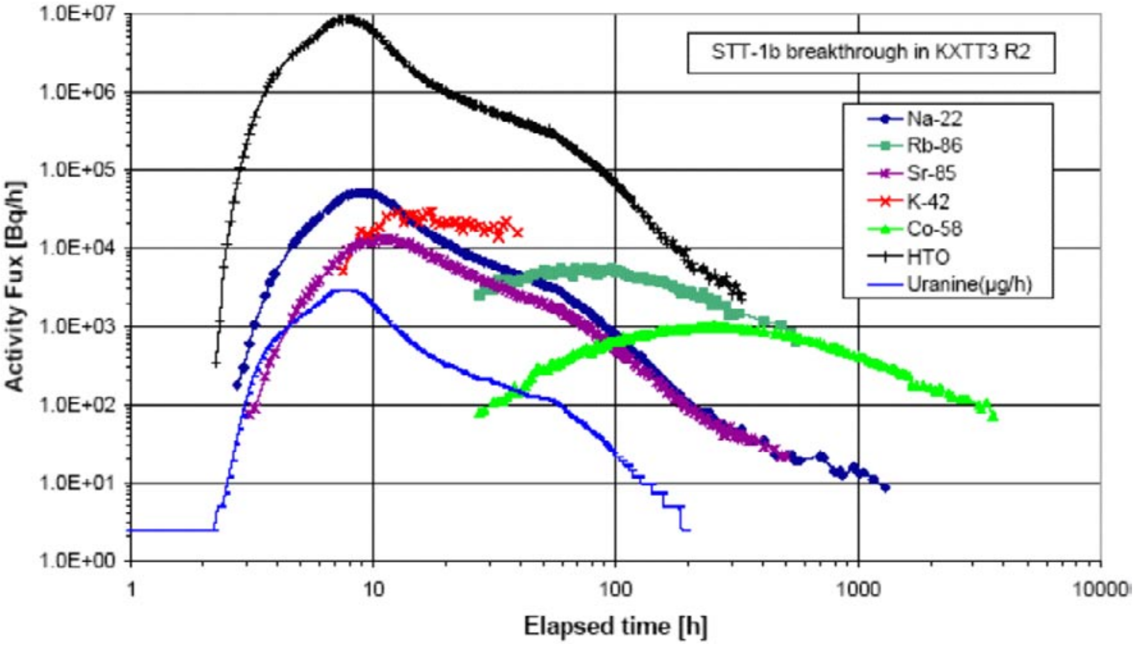

Figure 2-3. *Breakthrough curves from STT-1b /Andersson et al. 1999/.*

an acceptable fit to the experimental data, the modelling teams needed to modify their models and/or adapt the laboratory data. An evaluation of the modelling work in Tasks 4E and 4F has been presented /Elert and Svensson, 2001/ and an overall evaluation of Task 4 has been made by /Marschall and Elert, 2003/.

2.1.5 Material properties

This section presents an overview of the tracer transport and retention data provided as guidance to the modelling teams. The task specification emphasises that other data and information may be used provided that the motivation for the alternative values is given.

A modelling input data set (MIDS) has been derived containing sorption coefficients, effective matrix diffusivities, matrix porosity and density derived from laboratory experiments on Äspö diorite and material specific to Feature A /Winberg, 2000/. A summary of the values proposed for modelling is given in Appendix 1 of the Task 6A and 6B specification document /Selroos and Elert, 2001/.

Data on the porosity and diffusivity of mylonite and altered diorite sampled in the rim zone of Feature A /Byegård et al. 2001/ was available to the modelling teams in addition to laboratory data on gouge material from the experiments at the Kamaishi mine /Altman et al. 2000/.

Material properties for tracers not included in the MIDS data set have been compiled into an additional data set. These values are not based on experiments on Äspö material, but derived from other experimental studies and values used in safety assessments /Carbol and Engkvist, 1997; Ohlsson and Neretnieks, 1997; Vieno and Nordman, 1999/. The data is chosen to be representative of undisturbed rock.

2.2 Task 6A

The purpose of Task 6A is to provide a common basis for comparison in later Task 6 modelling exercises. It has therefore been defined to be applicable to both PA and SC models.

Task 6A is specified in /Selroos and Elert, 2001/. This task is concerned with the modelling of selected tracers used in the STT-1b test performed within the TRUE-1 programme /Andersson et al. 1999/. The test was made between packed off boreholes penetrating Feature A shown in Figures 1-3 to 1-5.

The STT-1b tracers modelled in Task 6A were ^{131}I, ^{85}Sr, ^{58}Co and ^{99m}Tc. Iodine is a non-sorbing tracer, while the others range from weakly to moderately sorbing.

In addition the strongly sorbing tracer ^{241}Am is included in the modelling task, although it was not used in the STT-1b test. The purpose is to study how the retardation of more strongly sorbing radionuclides can be extrapolated in time. However, in this case no comparison can be made with experimental data.

Radioactive decay is not considered in the modelling, and the injection concentrations have been corrected for decay. Simulations are performed up to a time of 10 years or until a full recovery is obtained for all tracers.

The following performance measures have been defined for Task 6A relating both to the measured injection curve and a Dirac pulse injection.

- Drawdown in injection and pumping boreholes (if available).
- Breakthrough time history for each tracer.
- Maximum release rate (Bq/a)
- The breakthrough times for the recovery of 5%, 50% and 95% of the injected mass (t5, t50 and t95).

2.3 Task 6B

The purpose of Task 6B is to identify and understand differences between the use of SC and PA models, and to study the influence of various assumptions made in PA calculations concerning extrapolation in time.

In Task 6B selected tracers used in the STT-1b test were modelled with new PA relevant boundary conditions and time scales /Selroos and Elert, 2001/.

In moving from SC to PA boundary conditions and time scales the modelling teams were expected to adapt their models in such way that the transport and retention processes are described in a relevant way. Any changes or assumptions should be explained and motivated.

The STT-1b test was adjusted to PA conditions with the following assumptions:

- In the TRUE-1 tracer experiments the gradient between the injection and pumping sections was in the order of 1, while in natural conditions a gradient of the order of 10^{-3} would be expected. Due to the change in gradient a water flow rate 1,000 times lower than in Task 6A is modelled. This can be achieved by different means, e.g. by changing the gradient or the pumping rate.

- The same flow path is assumed for Task 6B as in Task 6A, i.e. passive injection in KXTT1 R2 and withdrawal in section KXTT3 R2.
- The background head field observed during the TRUE-1 experiment should not be used, since it is assumed that the Äspö tunnel no longer causes a drawdown in Feature A. This may require changes in models and/or boundary conditions.

The tracers modelled in Task 6B are iodine, strontium, cobalt, technetium and americium, using both a constant injection (1 MBq/a) and Dirac pulse tracer injection boundary condition. The modelling input data set for Task 6A (see Section 2.1.5) also provides the basis for Task 6B. As with Task 6A, radioactive decay is not considered in the modelling. Simulations were requested up to 10^6 years or until a full recovery is obtained for all tracers.

The performance measures for both constant injection rate and Dirac pulse injection are the breakthrough time history for each tracer and the maximum release rate (Bq/a). Additional performance measures for the Dirac pulse injection are the breakthrough times for the recovery of 5%, 50% and 95% of the injected mass (t5, t50 and t95).

As different combinations of parameters/processes can reproduce the same breakthrough curves of STT-1b, but lead to different responses on PA time scales, one useful outcome of this study would be to identify important parameters/processes which need to be resolved in future field and laboratory experiments in order to distinguish between these alternative concepts.

2.4 Task 6B2

As with Task 6B, the purpose of Task 6B2 is to identify and understand differences between the use of SC and PA models, and to study the influence of various assumptions made in PA calculations concerning extrapolation in time. In particular, Task 6B2 investigates the effects of fracture heterogeneity.

Task 6B2 is specified in /Elert and Selroos, 2001/. In this task the boundary conditions used in Task 6B are modified to produce flow and transport over a larger area of Feature A. This is achieved by assuming that the tracers are injected and collected in fractures intersecting Feature A (see Figure 2-4).

As with Task 6B the modelled system reflects post-closure conditions where there is no tunnel causing drawdown, and water flow is governed by small natural gradients. The water flow in Feature A is assumed to be governed by the head difference between two fractures (X and Y) intersecting Feature A, positioned roughly where Feature B and NW-2’ are interpreted to intersect Feature A (see Figure 1-3). However, for the purpose of modelling the two fracture intersections have been assumed to be parallel in order to simplify the geometry (see Figure 2-5).

Injection is assumed to occur along a 2 m long line source overlapping the position of borehole section KXTT1 R2. The distance from the intersecting Fracture X to the injection line is 5 m. The flow will follow the general direction of the flow path used in STT-1b, i.e. from KXTT1 to KXTT3. However, in this case no pumping will occur in KXTT3. Tracer is collected in the upper intersecting Fracture Y, situated a distance of 10 m from the injection section.

As in previous tasks, the individual modelling teams in Task 6B2 were free to choose whatever conceptual model they thought appropriate. Unless otherwise stated, the specification is the same as for Task 6B. A key refinement is that the heterogeneity of the fracture surface characteristics can now have a more significant impact, and the data summarised below was provided to the modelling teams to support this.

The flow field in Feature A will be influenced by the heterogeneity of the transmissivity field. A compilation of the various hydraulic tests and their results is given in Chapter 5 of the final report of the first TRUE stage /Winberg et al. 2000/ indicating that a typical range of transmissivity for Feature A is 8 10^{-9} to 4 10^{-7} m^2/s. Very little information is available on the correlation length and anisotropy for the transmissivity, but /Winberg, 1996/ presents two-point statistical estimates of transmissivity data indicating a correlation length of about 0.3–0.4 m.

Compilations of two point statistics related to (hydraulic or physical) aperture relevant to Äspö and Stripa conditions show a span of reported practical ranges of approximately 0.005–0.1 m /Hakami, 1995/ and 0.05–0.2 m /Abelin et al. 1990/, for Äspö and Stripa conditions, respectively. Subsequent analysis by /Hakami and Larsson, 1996/ on a specimen from Äspö HRL, indicate practical ranges of 0.005–0.02 m. The lower bounds reported by /Hakami, 1995/ and /Hakami and Larsson, 1996/ fit with the practical ranges observed for the analysed samples from the pilot resin injection experiment, 0.003–0.005 m /Hakami and Gale, 1999/. Additional data on aperture distributions from artificially sheared fractures as well as measurements of grout injections are available from a granitic site in Japan. These data indicate that as displacement increases, elongated ridges and troughs in the fracture surface develop perpendicular to the direction of displacement. Furthermore, geometry data is available from excavation of a grout-injected fracture from a quarry in the western part of Japan. These data show a pattern with branching channels.

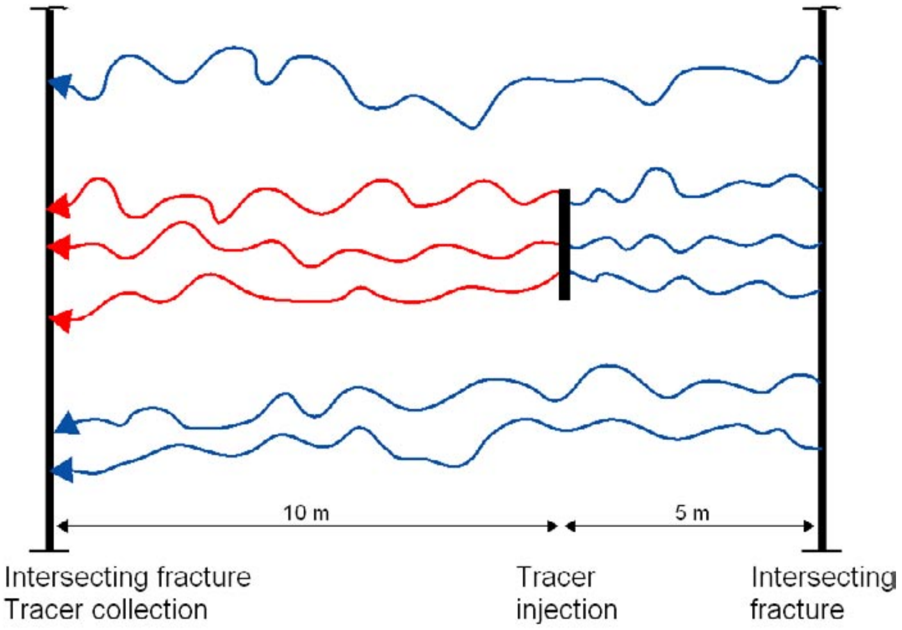

Figure 2-4. *Principle geometry for Task 6B2 seen in the plane of Feature A /Elert and Selroos, 2001/.*

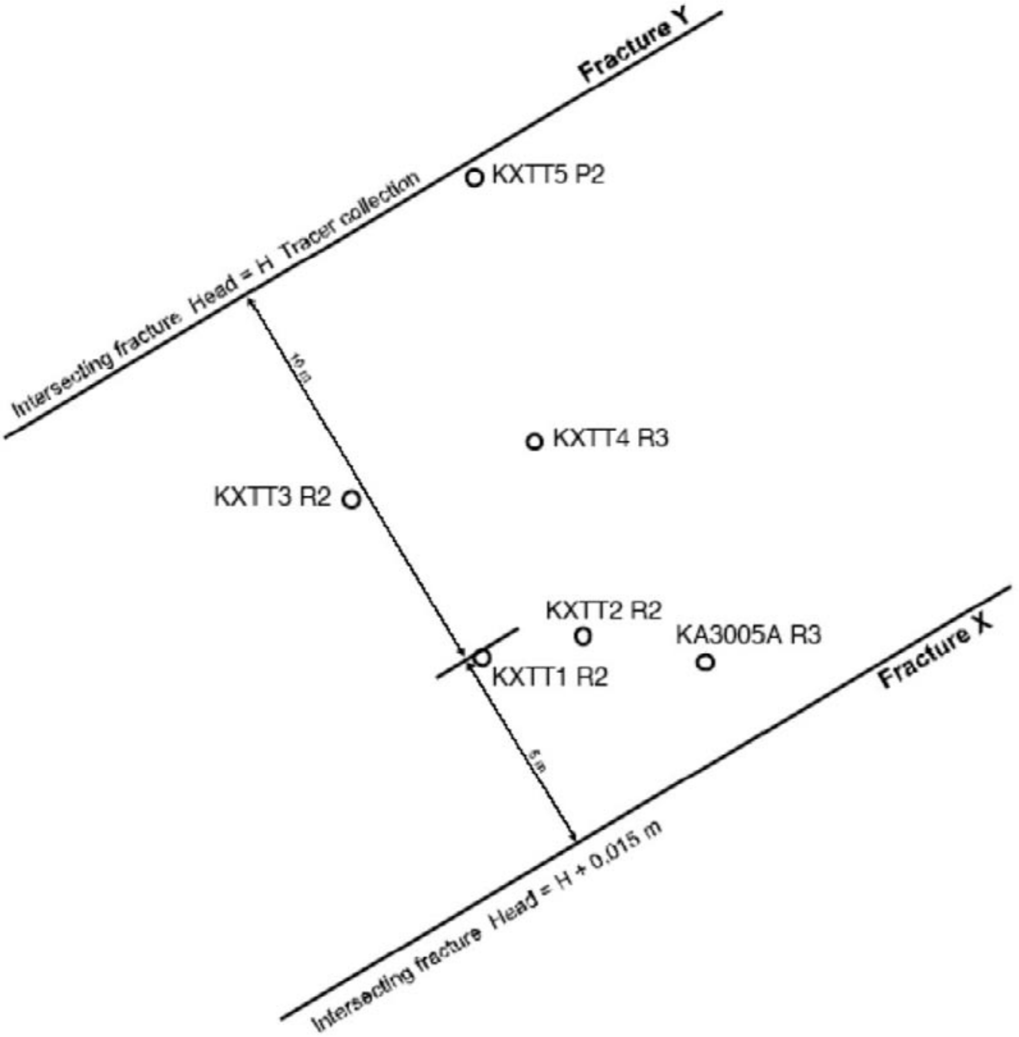

Figure 2-5. *Geometry of Task 6B2. Injection at line source at KXTT1 R2. Tracer collection at Fracture Y /Elert and Selroos, 2001/.*

The preliminary evaluation of the transport experiments performed on Feature A show, with a few exceptions, very similar transport parameters (dispersivity, accounting for all small scale heterogeneity; hydraulic aperture; and flow porosity). This finding indicates, at least from a transport perspective, that the studied part of Feature A shows a relative homogeneity as inferred from the investigated flow paths.

The breakthrough time history for each tracer for both a constant injection rate (1 MBq/a) and a Dirac pulse injection (unit input) is the primary performance measure for Task 6B2. Secondary performance measures are the maximum release rate and the breakthrough times for the recovery of 5%, 50% and 95% of the injected mass (t5, t50 and t95) for the Dirac pulse injection.

2.5 Review of task specifications

This section presents review comments on the task specifications, in particular addressing the questions.

- Do the specifications make sense?
- Are the objectives clear?
- Are the tasks well formulated?

2.5.1 Tracer test methodology

The radially convergent tracer test methodology has many useful attributes, not least that it maximises the possibility of collecting all the injected tracers. However, this approach confines the tracer pathway to a narrow strip which is likely to be the most conductive pathway and so may not be representative of the feature as a whole. Moreover, it doesn't provide a sound basis for Task 6B2 where predictions are required for a line source and sink. Thus in future experiments it might be useful to complement radially converging tracer tests with tests performed between borehole sections drilled within the plane of the feature. Also, it would aid the discrimination between models if tests were repeated for different flow rates.

2.5.2 Experimental data

As a familiarisation exercise, a review was carried out of the TRUE experiments and the associated site characterisation and interpretation /Winberg et al. 2000; Andersson et al. 2002a, 2002b; Poteri et al. 2002; Winberg et al. 2003/.

As a general rule, site characterization measurements aim to define a system geometry, then measure its hydrogeological boundary conditions and hydraulic behaviour, predict its transport behaviour and finally check these predictions with limited scale transport (tracer) experiments. This is the approach adopted by the TRUE experiments and a wide variety of measurement methods have been deployed to produce an impressive range, quality and quantity of site characterisation data. An excellent feature of the Äspö project is that these data have been comprehensively described and are available as reports, datasets and scientific publications.

One of the implicit assumptions of site characterization work is that there should be consistency when different types of measurement are interpreted. Hence, if a hydraulic test in a particular fracture is interpreted as occurring within a single channel then a subsequent tracer test interpretation should use the same geometry unless a different geometry can be explicitly justified. This consistency of interpretation serves two purposes, one is to give confidence that the overall construct of interpretations is reliable and the second is to enable the more penetrating site investigation techniques to serve as large scale predictors of more slowly measured behaviour. Hence, not all fractures identified by geophysics are hydrogeologically tested and parameterised and only a few identified hydrogeological features can be tested using tracers and probably only over a limited range.

The hydraulic testing involved in TRUE-1 appears to be comprehensive. It includes both steady-state and transient single-borehole tests and some cross-hole tests. As documented in Chapter 5 of /Winberg et al. 2000/, the tests on Feature A were based on intersections with 5 boreholes. Feature A appears to be reasonably isolated from the rest of the flow system, and connected over distances of about 10 m. However, detailed single borehole results shown in Figure 5-1 of /Winberg et al. 2000/ do not appear to reflect the idea of the borehole intercepting a single planar fracture. Rather Feature A appears distributed over intersection lengths in the order of 1 to 2 m (and sometimes more in the case of KA3005A). Furthermore, /Marschall and Elert, 2003/ report that there are indications from tracer tests, detailed flow logs and the Borehole Image Processing System that several flow paths exist within Feature A and that the presence of splays gives more than one intercept of Feature A in several of the boreholes. Bearing in mind that the in-feature tracer path lengths involved in the tracer test were in the order of 5 m, a simple 2D geometry seems unlikely. From this perspective the 3D flow interpretation of /Neretnieks and Moreno, 2000/ is not too surprising.

The results of the hydraulic tests are summarised in Table 5-5 of /Winberg et al. 2000/ and repeated in Table 2-1 of the Task 6B2 specification /Elert and Selroos, 2001/. The table indicates different transmissivities of different credibility dependent on different interpretation methods. The most important point is that each of the methods assumes a different geometry for the flow system. Also, in the case of the generalised radial flow (GRF) method the geometry can vary from test to test and potentially also in time (i.e. different geometry interpreted from different periods of the pressure versus time data). All these different geometries cannot simultaneously be correct interpretations.

Furthermore it is noted that other hydraulic test interpretations are possible, for example a preliminary examination of the data indicates that there may be a positive skin, which could be indicative of hyper-convergence in the test set up /Black et al. 2005/.

Hydraulic interpretation represents an important practical method of gaining confidence in up-scaling tracer test results to PA time and space scales, even though they are not directly analogous. The geometry of the flow test interpretations is currently too uncertain and this uncertainty is propagated throughout the tracer test interpretation and any subsequent PA style evaluation. In addition since all possibilities are retained in Table 2-1 of /Elert and Selroos, 2001/, it is possible that modelling groups could use parameters in their models that are not consistent (e.g. a value from a 3D analysis used in a 2D model).

A second aspect is the question of the region of test that gives rise to a specific interpreted result. In single borehole hydraulic tests, the ‘pressure signal’ radiates from the source point and encounters different obstacles/features that modify the spread of the signal. These changes are reflected back to the source point where pressure is observed so that the pressure versus time data represent, in a limited way, a form of increasing investigated region with increasing time. Pressure signals spread more rapidly than water-borne tracers and thus in general it can be inferred that the region investigated and interpreted in the hydraulic testing of TRUE-1 is very much larger than the region tested using tracers. This emphasises the care needed in constructing a logical system of up-scaling.

A major advance in the TRUE programme has been the characterisation of the internal structure of the main fault plane of Feature A. While Feature A is not necessarily representative of PA-scale paths, it provides a useful testing ground for understanding interactions between solutes and fractures.

2.5.3 Task 6 objectives

The Task 6 objectives (Section 1.5) are relevant, ambitious and challenging. It is difficult to see how they might be accomplished fully within a single project. This is primarily because Task 6 focuses on relatively short-term experiments, whereas to do justice to the objectives it would also be necessary to have access to information on long time scale phenomena for example from natural analogues and/or palaeohydrogeological studies. Thus perhaps the objectives should be modified so that they only relate to information that can be obtained from short-term experiments.

On the other hand, the objectives might legitimately be expanded with the aim of increasing confidence in the overall safety case for disposal, rather than just providing input to performance assessments. In this context a safety case is defined as /NEA, 1999/:

"... a collection of arguments, at a given stage of repository development, in support of the long-term safety of the repository. A safety case comprises the findings of a safety assessment and a statement of confidence in these findings. It should acknowledge the existence of any unresolved issues and provide guidance for work to resolve these issues in future development stages."

Thus a key element of a safety case is building confidence based on scientific evidence, rather than just relying on quantitative assessments of reasonable compliance with regulations. The extensive body of carefully produced tracer data and associated SC modelling together with the scrutiny provided by the Äspö Task Force helps to engender confidence in the safety case for disposal in hard rock. Moreover, this confidence is enhanced by the iterative approach to the TRUE experiments and their analysis.

2.5.4 Task 6 scope

As noted by /Benabderrahmane et al. 2000/, in many repository programmes the 50 to 100 m scale is key for geosphere retention, and it is right that Task 6 focuses on this length scale. Equally, understanding of radionuclide transport at this scale builds on experiments at the 5 to 10 m and laboratory scales, and thus it is good that the scope of Task 6 also includes the TRUE-1 experimental data set.

The well thought out and documented stepwise structure of Task 6, and the use of both experimental and PA boundary conditions, increases the likelihood that the primary objectives will be met. Also, the interaction of modelling teams from around the world undoubtedly provides opportunities for the sharing of ideas and experience to the benefit of the national programmes represented.

The background section of /Benabderrahmane et al. 2000/ contains an interesting discussion of differences between SC and PA models. While the points raised are correct, it might have been useful to have presented the discussion in terms of the fundamental reason for differences between SC and PA models. This is that SC models are designed to help understand the site in the relatively short term prior to closure of a repository, while performance assessments address longer term issues and therefore need to include slower processes. Furthermore, SC models need to represent phenomena and structures realistically, but models with pessimistic assumptions are often acceptable for PA purposes.

From this perspective, SC models may need to include short-term phenomena, in order to understand the results of short-term experiments. For example, kinetic sorption onto fracture infill and fracture surfaces could be important for understanding the TRUE experiments but unimportant for PA. In this regard, it is noted that such kinetic sorption has been used in the past to account for incomplete recovery of Sr^{2+} in a radially converging tracer test in a crystalline rock fracture zone /Hodgkinson and Lever, 1983/.

Performance assessments need to take account of phenomena occurring on long timescales. This can include changes in driving forces and water chemistry resulting from climate change or the evolution of the geosphere. Also, as noted by /Selroos and Elert, 2001/, different parts and aspects of the geological system become relevant for solute transport on different time and spatial scales. For the Task 6 modelling cases, solutes are transported within a relatively sparse network of relatively fast flowing features. However, on PA timescales, solutes are also likely to migrate through more slowly flowing features within the rock mass. Task 6 touches on this latter issue through the use of PA boundary conditions. However, it does not fully explore long time scale issues, and this limitation should be made clear.

2.5.5 Task 6A specification

/Selroos and Elert, 2001/ set out a clear and comprehensive modelling specification of Task 6A including a useful summary of the modelling input data set (MIDS) for tracer transport in Feature A. Moreover, reference is made to extensive and well-documented supporting reports where more detailed information can be found.

The specification is well formulated in that it both provides suggested conceptual models and parameters, thereby providing a starting point for the analysis, but also encourages the modelling teams to choose their own conceptual models and parameters, as long as these are suitably motivated and documented. This rightly focuses the effort on scientific understanding rather than just on the application of models.

In particular the discussion of information related to the geometry of flow paths is presented in such a way as to encourage alternative conceptualisations ranging from 1D to 3D flow. However, as noted in Section 2.5.2, it would have been beneficial if the flow geometry could have been constrained more tightly from a more comprehensive and consistent analysis of the hydraulic test results.

The deconvolution of tracer breakthrough curves to give the response curves for a Dirac pulse is a useful feature of the task specification, especially given the irregular shape of the injection profile. However, efforts aimed at producing a smoother experimental input profile should continue.

The specification contains a number of relevant numerical performance measures. However, it would also have been useful to specify some non-numerical outputs for the modelling team reports including a description of the conceptual and mathematical model, modelling strategy and data selection, numerical results, discussion and implications for the Task 6 objectives.

A potentially ambiguous part of the specification is that radioactive decay should not be included, but release rates are to be calculated in units of Bq/a. However, the modelling teams appear to have interpreted this unambiguously.

It is surprising that the modelling teams were not asked to predict tracer concentrations in the withdrawal borehole, in addition to the flux of tracer, as this would have provided a valuable constraint on the models in relation to the degree of dilution with water from elsewhere in Feature A and the surrounding rock mass.

2.5.6 Task 6B and 6B2 specifications

These cases are designed to allow a comparison to be made between PA and SC models and to study the influence of various assumptions made for PA calculations concerning extrapolation in time.

As with Task 6A these cases are described clearly and comprehensively. Moreover, it is commendable that the modelling teams are encouraged to make appropriate assumptions for PA modelling in order to explore the issues raised rather than just implement pre-defined conceptual models. For example in Task 6B2 there is the opportunity to explore different approaches to spatial variability.

One consideration regarding Task 6B2 from a PA perspective is that the head gradient drives water so that it moves solely through the near-planar Feature A. However in a PA context water is likely to also flow through other types of hydraulic features within the rock mass, including the averagely fractured rock. This needs to be borne in mind when drawing conclusions from this task about up-scaling in time.

2.5.7 Summary

Task 6 is based on an extensive and well documented hydraulic and tracer data set on two scales supported by extensive laboratory data. It addresses the important and challenging issue of how to bridge the gap between SC and PA modelling.

A range of possible interpretations of the hydraulic tests have been reported. They are based on different concepts and geometries and cannot all be correct. Consistency is required between the geometry assumed in analysing hydraulic and tracer tests.

A major advance in the TRUE programme has been the characterisation of the internal structure of the main fault plane of Feature A, which provides a useful testing ground for understanding the interaction of solutes with adjacent pore spaces.

It should be emphasised that the key difference between PA and SC models is the timescale over which phenomena are assessed. SC models may need to include short-term phenomena (e.g. kinetic sorption) in order to explain short-term tests. On PA time scales less permeable parts of the rock mass are likely to play a role and other long-term phenomena, including the evolution of the rock mass, need to be addressed. These points need to be borne in mind when drawing conclusions about PA from this study, especially in relation to the first objective to assess simplifications used in PA models.

The objectives of Task 6 are clearly stated and challenging. In addition to contributing to PA, the extensive body of carefully produced tracer data and associated SC modelling together with the scrutiny provided by the Äspö Task Force contributes directly to confidence in the safety case for disposal in hard rock. Moreover, this confidence is enhanced by the iterative approach to the TRUE experiments and their analysis.

A positive attribute of Task 6 is that modelling teams are encouraged to apply different conceptual models of varying complexity. This diversity will hopefully lead to a greater depth of understanding of transport in fractured rock.

The modelling specifications for Tasks 6A, 6B and 6B2 are well formulated and address the objectives of the overall study. Relevant numerical performance measures have been specified, but it would also have been useful to specify some non-numerical performance measures including the topics to be included in the Task 6 modelling team reports.

3 Modelling teams

3.1 Overview

Eleven modelling teams representing six organisations participated in this exercise, as shown in Table 3-1. Their work is documented in modelling team reports, and also in responses to a questionnaire concerning geometry, processes, parameters, numerical model and conceptual issues. This information is summarised in the first two sub-sections of Sections 3.2 to 3.12 for each modelling team in turn.

The final sub-section of Sections 3.2 to 3.12 presents an independent review of the work of each of the modelling teams, in particular addressing the following questions.

- Has the correct system been modelled?
- Has it been modelled correctly?
- What are the implications for the Task 6 objectives?

Table 3-1. Organisations and modelling teams participating in Tasks 6A, 6B and 6B2.

Organisation	Modelling team	Task 6A	Task 6B	Task 6B2
ANDRA	CEA	✓	✓	✓
ANDRA	Golder	✓	✗	✓
ANDRA	ITASCA	✓	✓	✓
CRIEPI	CRIEPI	✓	✓	✓
US DOE	Sandia	✓	✓	✗
JNC	Golder	✓	✓	✓
JNC	LBNL	✓	✓	✓
POSIVA	VTT	✓	✓	✓
SKB	CFE-SF	✓	✓	✓
SKB	KTH-ChE	✓	✓	✓
SKB	KTH-TRUE	✓	✓	✓

3.2 ANDRA-CEA

The theme of the work of the ANDRA modelling team from the Commissariat à l'Energie Atomique (CEA) was to identify the main flow and transport features and parameters for Feature A /Grenier, 2004/. This is viewed as a challenging task in view of the complex heterogeneity of the system and the relatively limited data. In particular the following issues, which are consistent with the objectives of Task 6, were addressed.

- Identification of the main flow and transport features for the experimental test regime.
- For the experimental test regime: characterisation of the parameter requirements, estimation of the level of information provided by the different tests and direct local measurements, characterisation of the level of uncertainties in the calibration phase and identification of system sensitivities.

- Development of a bridge towards longer time scales: determination of the mechanisms that operate under post-closure conditions, characterisation of the mobile and immobile zones, identification of related parameter requirements and how to determine them including the constraints provided by tracer tests.
- Development of PA models of reduced complexity, containing only the most important processes.

3.2.1 Approach

The full complexity of the system has not been included. Feature A was considered as a 2D plane with heterogeneity in the fracture plane accounted for by a dispersion tensor, which appears to be justified by the task specifications. In Tasks 6A and 6B a single one-dimensional flow channel was modelled, while for Task 6B2 unidirectional flow with a constant velocity was used.

The study focussed on matrix diffusion and sorption adjacent to the fracture and in particular on the heterogeneity of the pore spaces including the impact of the heterogeneity of retention properties, the extent to which they can be identified from tracer tests and the parameter requirements for the different regimes.

Three pore space models were used to investigate the impact of matrix diffusion heterogeneity (Figure 3-1). Model 1 is a simple deterministic homogeneous matrix model serving as a simple first step SC model and also as a PA model. Model 2 considers deterministic lateral heterogeneity with different matrix blocks as a function of distance from the fracture plane, as a representation of a Type 1 fault zone /Dershowitz et al. 2003/. A stochastic approach was used for Model 3, which considers heterogeneous matrix zones along the fracture with parameter values decreasing with depth.

The flow and transport equations were based on those presented by /Moench, 1989/ implemented within the mixed hybrid finite-element code Cast3M, and the numerical approach was verified against the analytical solutions of /Moench, 1989/.

3.2.2 Results and discussion

The implications of the ANDRA-CEA study have been summarised by /Grenier, 2004/ under the following headings.

Roles played by different matrix diffusion zones

- Short-term tracer tests explore the matrix zones in the close vicinity of the fracture due to limited contact times. In addition, only the higher diffusion and porosity zones result in significant retention. In Task 6A, gouge is the most important unit, together with the fracture coating and to a lesser extent cataclasite and mylonite.
- For slower flows in the post-closure regime, all zones considered are accessed by the plume with a penetration of tens of centimetres. The most diffusive zones are in equilibrium with the fracture for times short compared to the advective time, and can be efficiently modelled by a linear retardation term. In the less diffusive zones diffusion is transient, for example resulting in a long tail to the breakthrough curve.

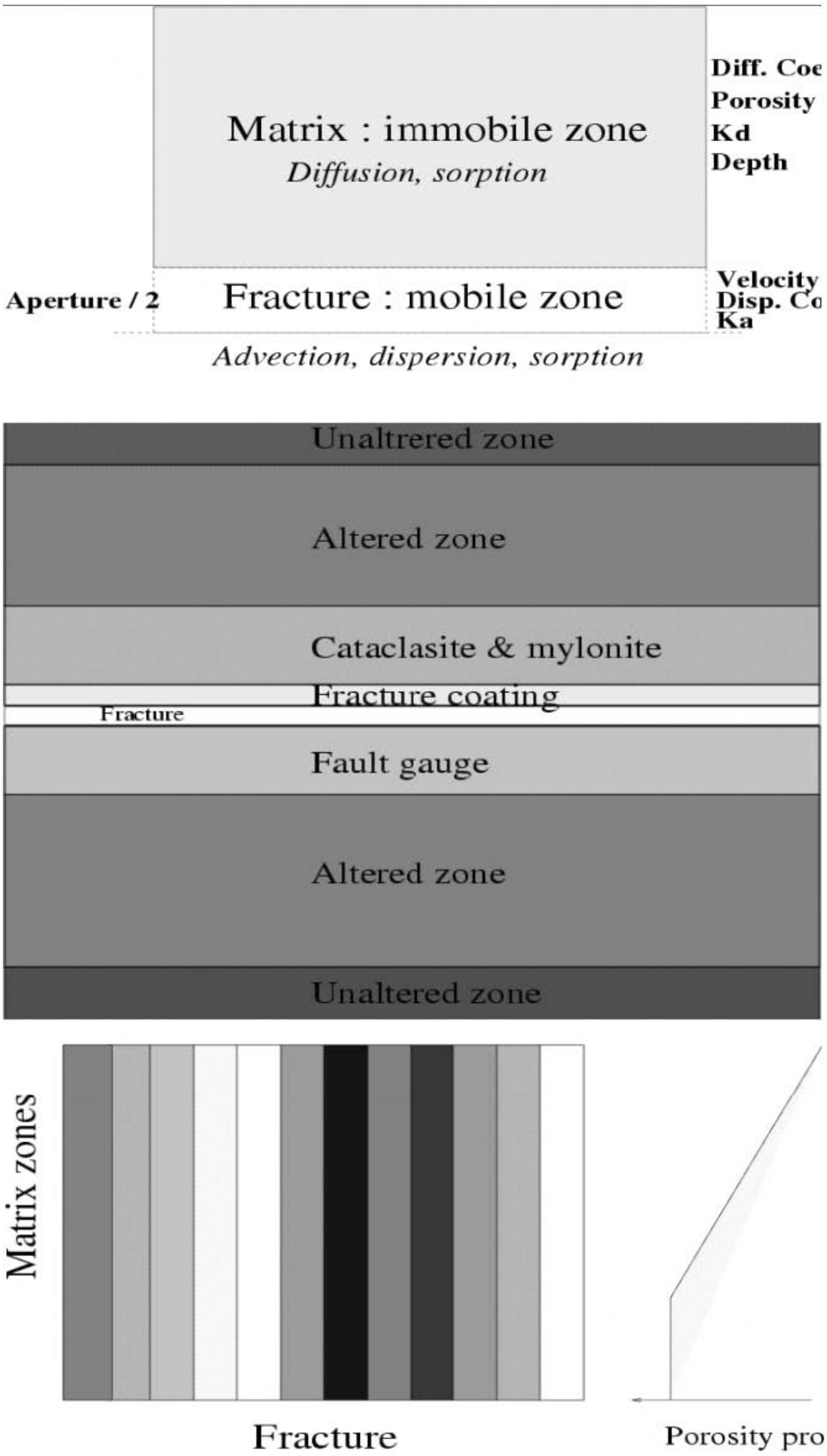

__Figure 3-1.__ The three pore space models considered by the ANDRA-CEA team: Model 1 (top): basic SC case considered and maximal level of simplification expected for PA model. Model 2 (middle): base case model considered for SC and PA cases. Model 3 (bottom): model considered to address the inverse problem and consequences of multi-calibration on PA scale predictions /Grenier, 2004/.

Construction of a simplified PA model

- It follows from the above analysis that Model 1 (Figure 3-1) is an appropriate approximation for PA, if equivalent parameters are used for the equilibrium and transient diffusion and sorption regions.

Constraining power of tracer tests

- As discussed above, tracer tests do not constrain the deeper and less diffusive matrix zones.
- Even for the matrix zones explored in tracer tests, the deduced parameters cannot be used directly in PA models.
- Thus tracer tests do not provide major inputs to the matrix zone parameters for use in PA models, and primary reliance should be placed on direct measurements of the relevant parameters.

Sensitivity

- In Tasks 6B and 6B2 the peak flux and its time of arrival are most sensitive to the depth, porosity and retention coefficient of the most diffusive matrix zones.

3.2.3 Review

The ANDRA-CEA team has carried out an interesting study of the implications of alternative matrix diffusion models. Their chosen conceptual and mathematical models are appropriate for the issues addressed, and confidence in the modelling results is enhanced by the verification against analytical solutions.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. Assess simplifications for PA: It is appropriate to use a simplified PA model consisting of a single matrix zone with equivalent parameters. The most significant parameters for the peak breakthrough under PA conditions appear to be the depth, porosity and retention coefficient of the most diffusive matrix zones.
2. Determine constraining power of tracer and flow tests for PA: Short-term tracer tests do not significantly constrain the matrix parameters required for PA models. In future it would be interesting to use relatively simple models, which have well-defined parameter groups, in conjunction with the ANDRA-Golder probabilistic sensitivity analysis approach (Section 3.3) to develop an understanding of constraints on effective parameter groups.
3. Support design of SC programmes for PA: Site characterisation programmes should include direct laboratory measurements of the transport properties of the intact rock matrix, and more detailed characterisation of flow paths.
4. Improve understanding using SC models: Model 2, which considers different matrix zones as a function of distance from the fracture plane, provides a useful SC representation of a Type 1 fault zone. This can be used to understand site-specific diffusion and sorption in Type 1 geological structures on different time scales, and to derive effective parameters for PA models. In future, further characterisation and modelling of the three-dimensional sub-structure of flowing features should be undertaken to improve understanding. In addition there is a need to validate the K_d approach under SC conditions.

3.3 ANDRA-Golder

The ANDRA modelling team from Golder Associates Oy focussed on the issue of the degree to which the tracer tests constrain rock mass properties within plausible ranges derived from laboratory and field data available prior to the tracer test /Holmén and Forsman, 2004/.

3.3.1 Approach

Task 6A

It was assumed that Feature A is a single fracture with a stochastically variable permeability field. A continuum approach was used for the calculation of the groundwater flow field and this was implemented in the GEOAN finite-difference code.

The well test was initially simulated for a large number of different realisations of the permeability field to identify those that have a flow near the tracer release point similar to the measured flow. Particle tracking was then applied to the identified realisations to derive a probabilistic distribution of the size and shape of the flow wetted surface area from the calculated plumes of tracer-contaminated water.

The transport processes (Figure 3-2) included were advection, dispersion, retardation, and exchanges with immobile storage zones (e.g. matrix diffusion). The retardation processes are represented by equilibrium partitioning between the fluid in the fracture and an infill

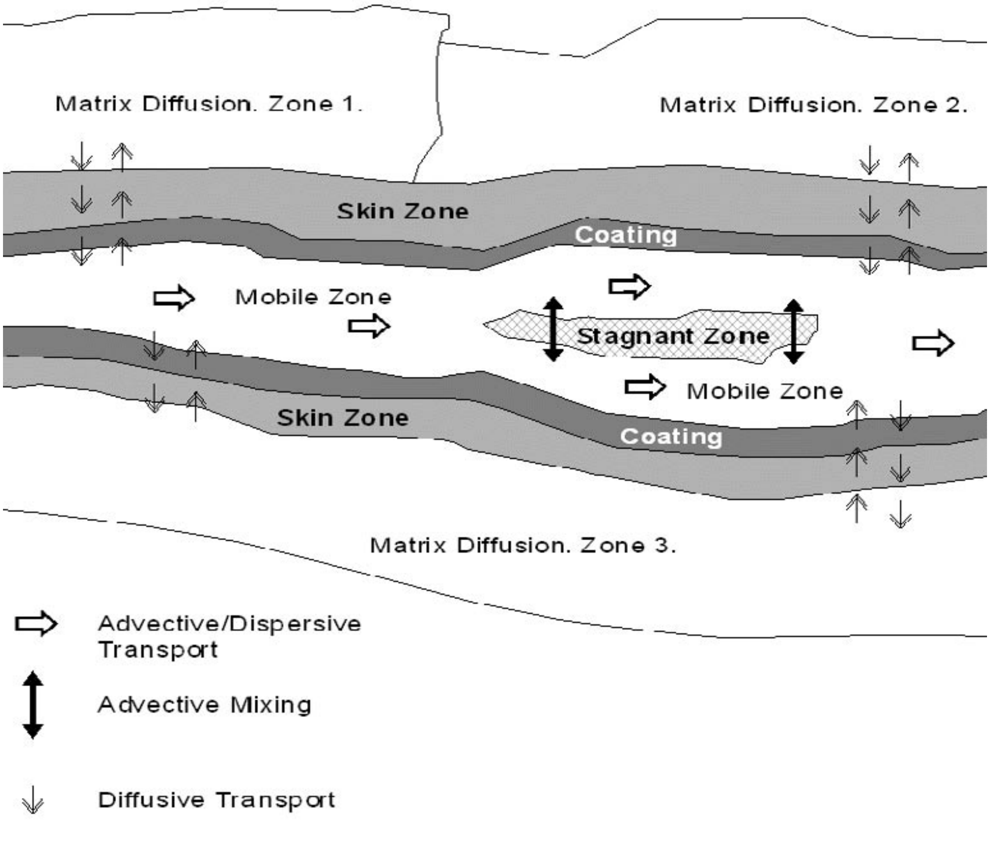

Figure 3-2. *A schematic cross-section along a pathway, showing examples of the features and processes that can be represented in the GoldSim Radioactive Transport Module used by the ANDRA-Golder team /Holmén and Forsman, 2004/.*

medium, fracture coating and skin zone, in addition to equilibrium partitioning between the diffusing fluid and the rock matrix. The diffusive interchanges with immobile storage zones along the main transport pathway are governed by matrix diffusion into immobile zones. The transfer rate into and out of the immobile storage zones is proportional to the concentration gradient and the diffusive properties of the zone. In addition a stagnant dispersive zone was included in which the interchange is proportional to the concentration difference and a transfer rate.

The transport modelling was carried out as a probabilistic sensitivity analysis using the GoldSim radionuclide transport module with uncertainties in transport parameters defined by probability distributions, and the injection concentration distribution set to the measured value. The simulated breakthrough curves that were found to match the measured breakthroughs were accepted and their parameter ranges compared with those of the input distributions to investigate the constraining power of the tracer tests.

The following sets of parameter distributions were derived for use in the Task 6B2 modelling.

- The given independent parameter distributions used as input data for Task 6A, based on the data given in the Task 6A and 6B specifications.
- The constrained independent parameter distributions based on the 89 accepted realisations for the strontium breakthrough curves.
- The constrained coupled parameter distributions consist of the ensemble of coupled parameter values as defined by the 89 accepted realisations. The difference is that for each of the 89 accepted realisations, a vector containing the combination of parameter values is retained, and thus the individual parameters are not independent. The overall probability distribution of the parameter values that takes place within the 89 accepted realisations are the same in the constrained independent parameter distributions and in the constrained coupled parameter distribution; the difference is that the parameters are uncorrelated for the constrained independent parameter distributions.

Task 6B2

Task 6B2 used the same flow medium, transport processes and modelling tools as Task 6A. Flow plumes between the release and interception lines were created for a large number of different realisations of the conductivity field.

In the first part of the analysis the entire plumes for the different realisations were analysed as single units. In the second part of the analysis the plumes were divided into 10 sub-plumes starting at equidistant regions along the release line in order to include the flow and velocity distribution within a plume in the transport model. In the transport modelling, GoldSim pipe elements were used to represents each of the sub-plumes. Correlations between the flow, length and flow wetted surface area of the sub-plumes was preserved using a bootstrapping method.

For each realisation of the transport model one of the stochastically-generated flow plumes was randomly selected and the flow properties of the GoldSim pipes were given by the properties of the sub-plumes. The transport properties were stochastically generated by GoldSim and were the same for all ten pipes. Equal amounts of tracer mass were injected into each GoldSim pipe, regardless of the flow in the pipe.

3.3.2 Results and discussion

Task 6A

The tracer tests with HTO and strontium were evaluated separately and combined, and it was found that 0.40%, 0.03% and 0.01% of the realisations respectively were accepted. In general the constrained independent parameter distributions were not significantly different from the given independent parameter distributions. However, a significant constraining power was demonstrated for the retardation factors of materials in direct contact with the flowing water (infill and fault gouge), but no constraining power for the materials not in direct contact with the flowing water (mylonite and diorite).

Compared to all the simulated breakthrough curves, the accepted breakthrough curves are characterized by earlier arrival times and higher peaks. Also, for strontium the following characteristics are preferred in the accepted realisations: large stagnant zone with small stagnant zone rate; small thickness of fault gouge; small K_d values for fault gouge and infill; large dispersivity.

The weak constraining power of the tracer tests demonstrated by the present analysis, and the good match to measured values, indicates that the tracer tests can be modelled using a large spectrum of parameter values, and that the key to finding the good match is to understand how the parameter values should be combined.

Task 6B2

Transport was modelled for the given independent parameter distributions, constrained independent parameter distributions and constrained coupled parameter distributions derived in Task 6A.

The parameter distributions that produced the most representative results for the TRUE-1 site was the constrained coupled parameter distributions since they were constrained by the tracer tests and include appropriate combinations of parameter values. The given parameter distributions represent reasonable ranges, but as they are not constrained by the results of the tracer test, and they generally produce a much later arrival of the mass than the constrained coupled parameter distributions.

In Task 6B2, the slower flow increases the relative retardation of strontium compared to HTO, from the value of 1.7 in Task 6A. For the Dirac pulse and the constrained coupled parameter distributions, it was found that the relative arrival time of the strontium and HTO peaks in Task 6B2 was approximately 27.

The interaction of the tracers with rock masses not in direct contact with the flowing water is an important process on PA time scales. The properties that control these processes are not well constrained by standard tracer tests and thus direct measurements of these properties are required.

Implications

Traditionally when using SC data for deriving plausible ranges of parameter values, the objective is to derive probability distributions of the relevant parameters. It is also often assumed that these distributions are independent and not correlated to each other, or some uncertain correlation is introduced between a few parameters.

The basic problem is that flow and transport models incorporate a large number of parameters, and credible fits to test results can be achieved with many different combinations of those parameters. Thus, testing can not be expected to produce definitive values of the parameters, or even useful probability distributions for them. The uncorrelated probability distributions are not very useful because it is the specific combinations of parameter values that succeed or fail to match tests. In other words, the analysis of the tests will result in extremely complex joint probability functions for the entire suite of parameters.

The generation of random realisations, based on a set of plausible (given) parameter distributions, and keeping only the realisations that produce an acceptable match to the tracer test data, is an informal Bayesian approach to mapping the entire joint probability density space and converting from prior to updated probabilities. In this way it has been possible to derive constrained parameter distributions. The constrained independent distributions are, however, not necessarily very useful (as discussed above). Therefore constrained coupled parameter distributions have been derived.

The constrained coupled parameter distributions consist of the ensemble of coupled parameter values as defined by the accepted realisations. The difference is that the individual parameter values are combined according to the parameter combinations that resulted in the accepted realisations.

The use of the constrained coupled parameter distributions for the PA modelling will produce better predictions with smaller uncertainties than the use of the constrained parameter distribution, because the correct parameter correlations are included. This is an important improvement compared to an assumption of independent parameters or the inclusion of some uncertain and limited correlation between a few parameters.

This might have important implications for how PA analyses should be carried out. The approach, in which one tries to establish independent distributions for each parameter, possibly with some correlations, is not necessarily the best approach, as it may be nearly impossible to integrate the knowledge gained from different field-tests into such distributions.

Instead, the approach used in this study is proposed, namely:

1. Use as much general data as possible to develop the given (prior) parameter distributions (with possible correlations).
2. Use the given parameter distributions as input data for SC modelling. Only realisations that produce an acceptable match to field test data sets, considering one or several tests, should be propagated to the PA modelling. To improve the efficiency of the process of finding the acceptable realisations, constrained parameter distributions can be derived and these distributions can be used instead of the given distributions as input data for the SC modelling. In a wider perspective, more complex modelling can be carried out and the field test data, against which the modelling results are matched, may not only come from tracer tests but could also be taken from other tests and analyses, e.g. pump tests, laboratory analyses of chemical properties etc.
3. PA modelling for the specific combinations of parameter values that pass all tests against field data (the constrained coupled parameter distributions).

3.3.3 Review

The probabilistic approach applied by the ANDRA-Golder team provides a refreshing alternative perspective on the investigation of the constraining power of tracer (and other) tests, and has important implications for probabilistic PA studies. A traditional problem with probabilistic analyses is that correlations between parameters are ignored, or given little consideration, and in consequence implausible and inconsistent parameter combinations are used and the uncertainty in predictions is increased. The approach advocated in this study is a practical way around this problem. It would be useful to analyse the accepted realisations to look for clusters of similar cases representing relatively discrete conceptual models, which could then be propagated separately through the PA. Also, as in the JNC-Golder analysis (Section 3.7) it would be good to analyse for parameter groups.

The approach provides a complementary perspective to deterministic analyses, and it is encouraging that similar conclusions are drawn about the interaction of tracers with material at different distances from the flowing water on experimental and PA time scales.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. Assess simplifications for PA: The interaction of the tracers with matrix zones not in direct contact with the flowing water is an important process at PA time scales but the relevant properties are not well constrained by standard tracer tests and thus direct measurements of these properties are required.
2. Determine constraining power of tracer and flow tests for PA: Short-term tracer tests do not significantly constrain the uncorrelated parameter distributions. It is the specific combinations of parameter values that succeed or fail to match tracer tests. Thus correlations between parameters need to be included, and a practical method of achieving this has been proposed.
3. Support design of SC programmes for PA: Site characterisation programmes should include direct measurements of the transport properties of the different matrix zones.
4. Improve understanding using SC models: The tracer interaction model (Figure 3-2) includes zones with a range of characteristics reflecting the detailed conceptual model of Feature A, which can be used to understand site-specific diffusion and sorption on experimental and PA time scales.

3.4 ANDRA-ITASCA

The ANDRA modelling team from ITASCA Consultants /Billaux, 2004/ had not previously participated in the Äspö Task Force and thus an initial aim of their work was to gain an understanding of Feature A through Task 6A. This resulted in some questions relating to conceptual model uncertainty.

3.4.1 Approach

The ANDRA-ITASCA team considered Feature A as planar with a network of one-dimensional flow channels representing the flow field. The in-plane aperture is heterogeneous in several senses. First, channelling in itself is a representation of preferential flow paths, i.e. of a heterogeneous plane. Secondly, the properties of the individual flow channels such as orientation, length, and conductivity/aperture are taken from statistical distributions. Because of the assumed complete mixing at channel intersections, there is heterogeneity of the tracer paths. For example, even in the radially converging test flow field the tracer will follow several paths.

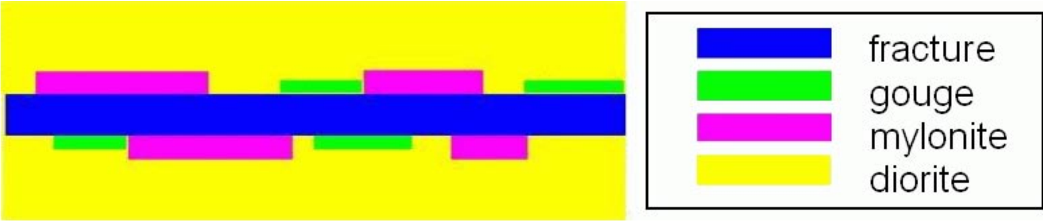

Figure 3-3. *Immobile pore spaces in the ANDRA-ITASCA conceptual model /Billaux, 2004/.*

Calibration of the model started with the geometry of the network, and then dealt with the channel conductivity distribution. The network was made slightly anisotropic, with channel lengths and density such that the average 1D length between intersections was close to the indicated correlation length. A highly conductive zone was introduced between KXTT2 and KXTT3 in order to simulate the hydraulic head responses of these two boreholes.

The immobile pore space was represented by gouge, mylonite and diorite zones where the tracer diffuses normal to the channels (Figure 3-3). The diorite is present everywhere next to flow channels, but may be separated from them by some thickness of gouge or mylonite. The rationale for this is that it endeavours to represent the conceptual model shown in the specification (Figure 1-5) with the smallest number of components. Also, dead-end channels were retained within the model as a representation of stagnant zones.

The modelling was performed within the framework of the Advection-Dispersion-Diffusion (ADD) equation where the processes contributing to the shape of breakthroughs are advection, longitudinal dispersion, mixing at intersections, adsorption on channel sides, diffusion into the immobile pore space, and adsorption in the pores of the immobile pore space.

Non-sorbing tracer breakthrough was then used to calibrate the flow/velocity relationship through the choice of a conductivity/aperture law. The dispersion coefficient and matrix diffusive properties were then chosen, firstly by using the values given in the specifications and then modifying them to improve breakthrough calibration. The final stage of the calibration process concerned the sorbing tracer breakthrough curves. K_d's and K_a's were chosen for the various materials and tracers, keeping the values as close to the values in the specification as possible.

Tasks 6B and 6B2 used the same model as Task 6A with the exception that after computing the flow due to the changed boundary conditions, the system was simplified by removing all channels which are not located downstream of the injection well or injection line, and upstream of the recovery well or recovery line.

Calculations were performed using the 3FLO code /Billaux and Paris, 2001/, which uses the discrete parcel random walk approach to solve the transport equations.

3.4.2 Results and discussion

The ANDRA-ITASCA team consider that the ADD equation has not been proved sufficient for the problem of estimating properties on experimental time scales and then extrapolating to PA time scales. First, on the experimental time scale, it was necessary to assume that

Co samples a different flow field from Sr and I in order to calibrate the Co breakthrough. This indicates that some of the physics may have been overlooked. Secondly, two fits for Sr with and without matrix diffusion yield extreme differences in the predictions for Tasks 6B and 6B2.

Compared to these large conceptual uncertainties, the variability in predicted response from realisation to realisation is quite small.

3.4.3 Review

The statistical channel network model used by the ANDRA-ITASCA modelling team provides a useful alternative perspective on modelling heterogeneity within Feature A, although it appears that the variability between realisations was quite small. It is interesting to note that acceptable fits to the tracer test data could be found with no matrix diffusion. Presumably, the various in-plane dispersion terms were able to simulate similar behaviour on short time scales. However, models with and without matrix diffusion lead to very different predictions on PA time scales. Thus the ANDRA-ITASCA team have provided a useful reminder that considerable conceptual uncertainties remain even on relatively short time and length scales.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** There remains conceptual uncertainty about the key processes to be included in PA models.
2. **Determine constraining power of tracer and flow tests for PA:** Reasonable fits to short-term tracer tests can be found with and without matrix diffusion and thus these tests alone do not significantly constrain the conceptual model for transport.
3. **Support design of SC programmes for PA:** Relevant laboratory data is required in addition to tracer tests.
4. **Improve understanding using SC models:** The statistical channel network approach is potentially useful for understanding flow within Feature A, but further information on the channel statistics is required.

3.5 CRIEPI

3.5.1 Approach

The CRIEPI modelling team /Tanaka, 2004/ considered Feature A to be a single fracture containing some fault gouge, surrounded by Äspö diorite with an altered rim zone either side of the fracture (Figure 3-4). Advection, dispersion and surface sorption were considered within the fracture. Matrix sorption was considered in the fault gouge, while in the altered and unaltered Äspö diorite advection, dispersion, matrix diffusion and sorption were considered. The Galerkin finite-element codes, FEGM and FERM /Kawanishi et al. 1987/, were used for groundwater flow and solute transport respectively.

The transmissivity distribution was spatially correlated, with parameters identified on the basis of the drawdown during several tracer tests. A constant fracture transport aperture was assumed with a value determined through numerical simulation of tracer test STT-1b.

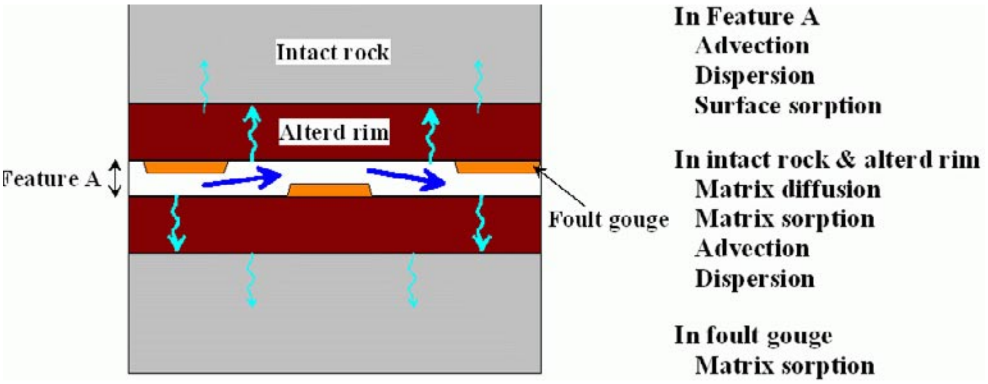

Figure 3-4. *Schematic view of the geometry and processes considered by CRIEPI /Tanaka, 2004/.*

In general the transport parameter values, including surface sorption coefficients, porosities, pore diffusivities and rock matrix distribution coefficients were taken from the task specification document. However, the fault gouge distribution coefficients for strontium and cobalt were calibrated through simulations of STT-1b.

Three-dimensional finite-element grids were used, extending 0.1 m into the matrix. In addition, Task 6B2 also considered one-dimensional flow in the fracture with diffusion and sorption perpendicular to the fracture.

3.5.2 Results and discussion

The CRIEPI analysis confirmed that advection was the most prominent process in Task 6A and matrix diffusion was the most prominent in Tasks 6B and 6B2. The significant technical achievements in Task 6A were the estimation of the transmissivity distribution, fracture aperture, and gouge sorption coefficients. For Tasks 6B and 6B2 the significant technical achievement was the estimation of sorption coefficients for the altered rim and intact rock.

The CRIEPI modelling team considered that there is no particular problem in using the conventional advection-dispersion-diffusion approach and that the primary problem is to estimate the parameters accurately. In particular, in order to improve the reliability of performance assessments it is important to have a reliable method for estimating transport properties, especially surface and matrix sorption coefficients, from the results of in-situ tracer experiments and laboratory tests. Also the CRIEPI team considered that irreversible sorption needs to be included in order to model the migration of some radionuclides such as cobalt.

In Task 6B2 the breakthrough curves obtained by using the one-dimensional model were very different from those using the three-dimensional model.

3.5.3 Review

This was the only study that explicitly included advection and dispersion in the altered rock matrix in the 3D models, and this probably accounts for the different results for the 1D model in Task 6B2.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** One-dimensional models are often used in PA and thus it is important to fully understand the differences between the 1D and 3D calculations for Task 6B2.
2. **Determine constraining power of tracer and flow tests for PA:** Not addressed.
3. **Support design of SC programmes for PA:** Irreversible sorption may need to be considered in SC programmes.
4. **Improve understanding using SC models:** The use of a 3D finite-element model, including the altered rock region, has the potential to model the detailed sub-structure of features if suitable small scale characterisation data becomes available.

3.6 DOE-Sandia

Due to resource constraints the US DOE modelling team from Sandia National Laboratories was not able to complete its participation in Tasks 6A and 6B. In the absence of a modelling team report, the information in this section is based on their questionnaire responses.

3.6.1 Approach

Feature A was modelled as a single fracture with an isotropic heterogeneous transmissivity distribution modelled using a multi-Gaussian random field conditioned to the five hydraulic tests. Advection, dispersion and matrix diffusion were modelled for all tracers. In addition, surface sorption was also modelled for Tc and Am. A single streamline was considered for each transport calculation with a Gaussian longitudinal dispersion length of 5 percent of the travel distance.

The conceptual model of the considered matrix zones is shown in Figure 3-5. However, the various zones were not modelled explicitly. Instead they were modelled with a multi-rate model with a continuous log-normal distribution of mass transfer rate coefficients. The diffusive capacity was assumed to vary with mass-transfer rate as illustrated in Figure 3-6. It is noted that in contrast to some PA models, the diffusive capacity is finite in this approach.

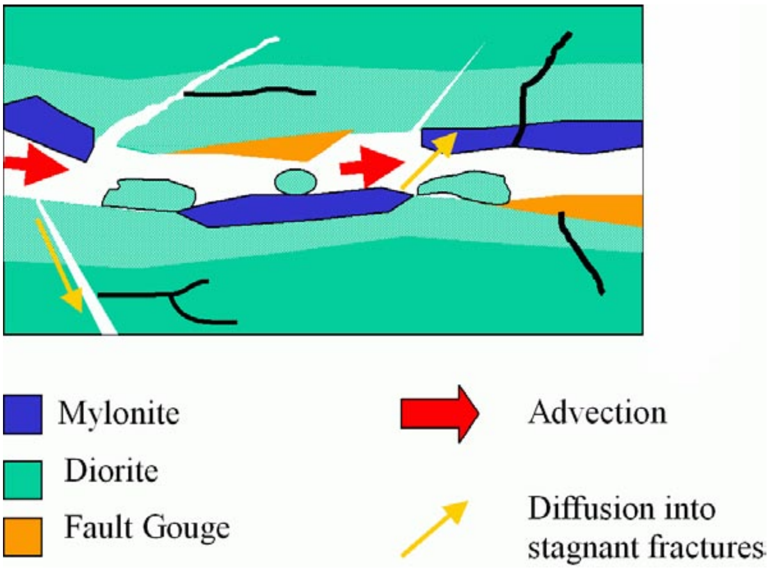

Figure 3-5. *DOE-Sandia conceptual model.*

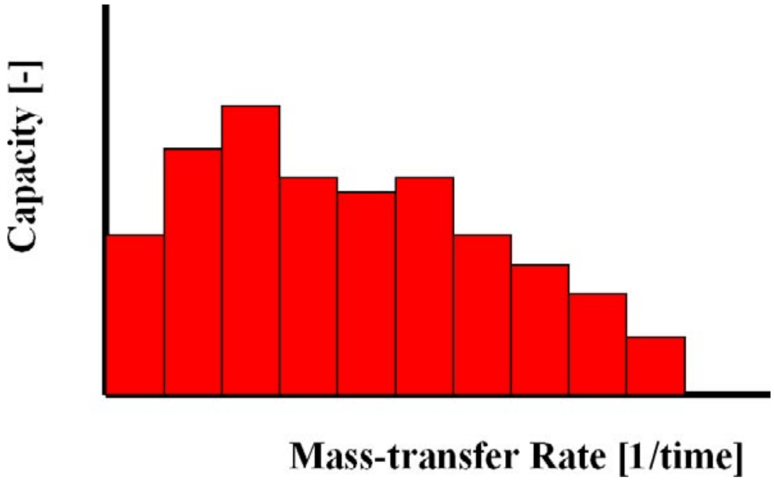

Figure 3-6. *Diffusive capacity as a function of mass-transfer rate for the DOE-Sandia multi-rate model.*

The transport equations were solved using a semi-analytical Laplace transform technique. The transport parameters were up-scaled by assuming a constant relation of the mean diffusion rate to flow velocity. Thus the decrease in velocity by a factor of 1,000 in Task 6B was coupled with a decrease in the diffusion rate by the same factor. This is not a unique assumption and the Sandia team plan to explore other up-scaling assumptions in future work, including assuming a constant Damkohler number.

The transport parameters were estimated by inverse modelling of the STT-1b tracer test and from laboratory data. Uncertainty was addressed using Monte Carlo simulation.

3.6.2 Results and discussion

No final results reported.

3.6.3 Review

The DOE-Sandia team has provided an innovative perspective on possible relationships between the properties of the matrix zones and the up-scaling of transport parameters. However, justification needs to be given as to why the mean diffusion rate was up-scaled assuming a constant relation to the flow velocity. If the work is carried forward, it has the potential to provide a useful way of summarising a range of matrix zone data, and facilitating its transfer to other situations.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** The proposed model has the potential to provide a link between PA and SC matrix diffusion models, although further validation studies are required to confirm this.

2. **Determine constraining power of tracer and flow tests for PA:** If the distribution of diffusive rates and capacities can be shown to have some universal validity then this approach could facilitate the process of linking matrix parameters determined in tracer tests and those measured for intact rock.
3. **Support design of SC programmes for PA:** Not addressed.
4. **Improve understanding using SC models:** Not addressed.

3.7 JNC-Golder

The JNC modelling team from Golder Associates Inc. performed integrated SC and PA modelling /Dershowitz et al. 2004/ using the GoldSim PA code /Miller, 2002/ and the MAFIC/LTG SC code.

JNC's objectives for Task 6 are to:

- Identify key assumptions needed for long-term prediction in PA and identify less important assumptions in PA.
- Identify the most significant PA model components of a site.
- Prioritise assumptions in PA modelling and demonstrate a rationale for simplifications in PA models by parallel application of several PA models of varying degrees of simplification.
- Provide a benchmark for comparison of PA and SC models in terms of PA measures for radionuclide transport at PA temporal and spatial scales.
- Establish how to transfer SC models using site characterization data to PA models, i.e. how to simplify SC models into PA models in a consistent manner.

This work focussed on evaluating the extent to which the parameters that are determined from SC experiments constrain solute transport at PA time scales.

3.7.1 Approach

The goal of the JNC-Golder team was not to determine the single "correct" set of transport pathway properties. Rather, a stochastic sensitivity study was carried out to determine the extent to which the TRUE-1 tracer breakthroughs constrain the tracer pathway properties. In effect, how much is the space of physically possible transport parameters decreased by the results for the STT-1b tracer experiments?

The conceptual transport model used for Task 6A is illustrated in Figure 1-5 and Figure 3-7. The GoldSim model includes advection, longitudinal dispersion, diffusion to immobile zones, and transfer between advective and stagnant zones within the fracture plane together with linear equilibrium sorption/desorption for each immobile zone.

The evaluation of the power of site characterization experiments to reduce uncertainty requires an understanding of the level of uncertainty before the experiment. This was defined in terms of distributions, and minimum and maximum values for the physically possible range of transport parameters based on /Mazurek and Jacob, 2002/ and /Winberg et al. 2000/. By comparing the breakthrough curves obtained from each GoldSim realisation against the measured breakthrough curves, the parameter uncertainty was then reduced by only considering those parameters and parameter combinations which provided a good match.

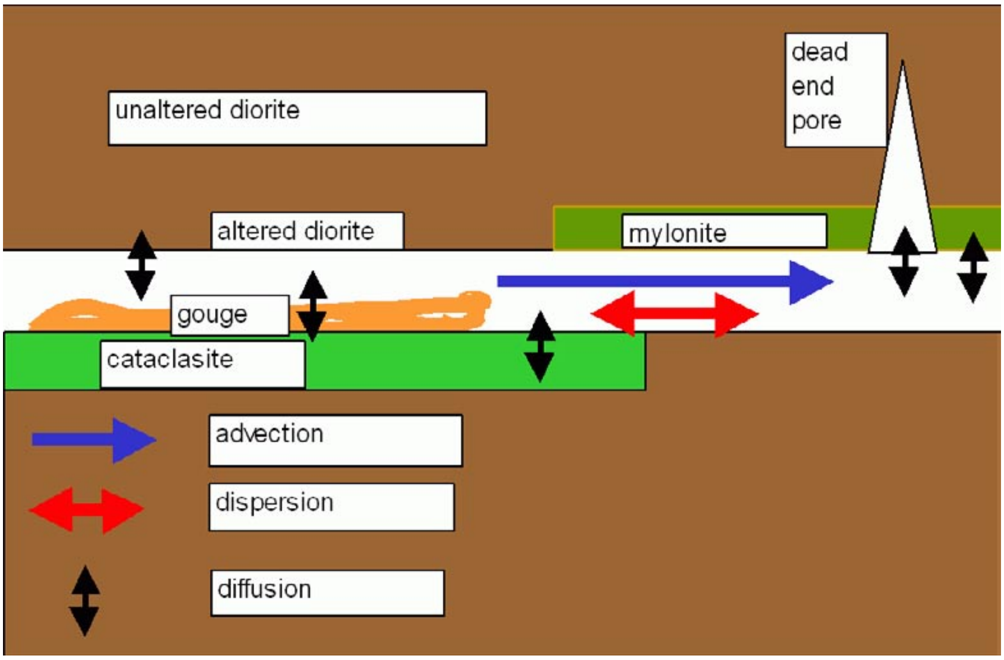

Figure 3-7. *Illustration of the JNC-Golder conceptual model /Dershowitz et al. 2004/.*

Task 6B was run using three realisations which were conditioned to ^{85}Sr tracer breakthrough on the experimental time scale. In Task 6B, the experimental determination of transport and immobile zone parameters was propagated to a PA time scale model. However, on PA time scales, the immobile zone parameters for the rock mass dominate, whereas the rock mass immobile zone parameters are completely unimportant at experimental time scales.

The JNC-Golder strategy for Task 6B2 focussed on how transport is influenced by different hypotheses regarding the in-plane heterogeneity of Feature A. Task 6B2 simulations were carried out using a discrete fracture stochastic continuum code, FracMan/EdMesh, to generate 2D heterogeneous realizations of Feature A, and MAFIC/LTG to solve solute transport in 2D with multiple immobile zones. The micro-structural conceptual model used for transport in Task 6B2 was similar to that used for Tasks 6A and 6B with some modifications, primarily resulting from modelling of the heterogeneous 2D flow field.

Two sets of simulations were carried out for Task 6B2. The initial simulations used the same 1/1,000 advective velocity used in Task 6B to approximate PA conditions, but set the downstream boundary condition as a line sink, representing the effect of an intersecting fracture. In the second set of simulations the specified boundary conditions were used.

3.7.2 Results and discussion

The simulations carried out for Task 6A clearly demonstrated the degree of residual uncertainty in immobile zone parameters following conditioning to conservative and sorbing tracer experiments. Conservative tracer experiments were found to provide a poor constraint on the micro-scale immobile zone parameters, which determine sorbing tracer breakthrough. Conditioning to sorbing tracer experiments provides a much better constraint. However, uncertainty in immobile zone parameters, which are unimportant for weakly sorbing tracers, can propagate to larger uncertainties in more strongly sorbing tracer breakthrough. Task 6A simulations determined that while the physical parameters of solute transport were not well constrained, parameter groups such as the F-factor (β parameter) and the mobile/immobile volume ratio were constrained.

The Task 6B simulations illustrate the power of the use of stochastic simulation and sensitivity studies to quantify the residual uncertainty at PA time scales based on models conditioned to in situ experiments. Further refinement of the conditioning to sorbing tracers at the experimental time scales would not improve the conditioning for the rock mass immobile zone which dominates at the PA time scale. Thus Task 6B demonstrated that the residual uncertainty from site characterization does propagate to significant uncertainty at PA time scales. This is particularly true for parameters such as the available immobile zone porosity of the rock mass, which is not constrained at SC time scales.

In Task 6B2 the change in boundary conditions can have a significant influence on the propagation of uncertainties from the SC to PA scales. However, preliminary simulations indicate that the added uncertainty due to two-dimensional flow is less significant than other uncertainties addressed in Task 6B.

3.7.3 Review

The stochastic sensitivity study carried out by the JNC-Golder team using an integrated SC and PA approach provides a comprehensive approach to addressing the Task 6 objectives. For example, it stresses the importance of accounting for residual uncertainty in transport parameters rather than propagating best-fit parameters to site characterisation data to PA predictions.

An important result from the Task 6A simulations was that while the physical parameters of solute transport were not well constrained, parameter groups such as the mobile/immobile volume ratio were constrained.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** The degree of complexity of the GoldSim transport model appears to be adequate for PA calculations along a single pathway. However, the uncertainty in how to justify a model for the distribution and connectivity of these pathways remains.
2. **Determine constraining power of tracer and flow tests for PA:** Residual uncertainty from site characterization propagates to significant uncertainty at PA time scales, in particular for the available immobile zone porosity of the rock mass, which is not constrained at SC time scales.
3. **Support design of SC programmes for PA:** Site characterisation programmes should include direct measurements of the transport properties of the intact rock matrix.
4. **Improve understanding using SC models:** Considerable uncertainty remains in the SC conceptual model of Feature A, which can only be resolved by more data.

3.8 JNC-LBNL

The work described in this section was performed by a temporary additional modelling team from the Japan Nuclear Cycle Development Institute (JNC) and the Lawrence Berkeley National Laboratory (LBNL) /Doughty and Uchida, 2004/.

3.8.1 Approach

The key flow and transport processes occurring in a complex fracture zone such as Feature A are assumed to be advection, dispersion, diffusion, and sorption. The key factors affecting how and where these processes occur, illustrated in Figure 3-8, are spatial permeability variations over the plane of the fracture zone (the x-y plane in Figure 3-8); multiple sub-fractures within the fracture zone thickness (the z direction in Figure 3-8, where two sub-fractures are shown); gouge materials within each of the sub-fractures; splays, or minor fractures, in between the two sub-fractures that break up the rock into blocks of sizes a fraction of the width of the complex fracture; dead-end pores and splays into neighbouring rocks; and unaltered rock surrounding the fracture zone.

The JNC-LBNL team applied a new modelling approach that has recently been developed to model these processes in complex fracture zones /Tsang and Doughty, 2002/.

A two-dimensional (2D) heterogeneous fracture-transmissivity distribution was generated and the 2D flow field, q(x,y), was calculated with a finite-difference code. The structure in the third dimension (the fracture zone thickness) was accounted for by assuming that there are two sub-fractures in a ladder-like structure (Figure 3-8). It was assumed that at each (x,y) location: (i) the flow q(x,y) represents the sum of the flow in the two sub-fractures: $q_1 + q_2 = q$; (ii) q, q_1 and q_2 are in the same direction; and (iii) the ratio of flow between sub-fractures 1 and 2 is $\alpha = q_2/q_1$, where the parameter α is denoted the fracture structure

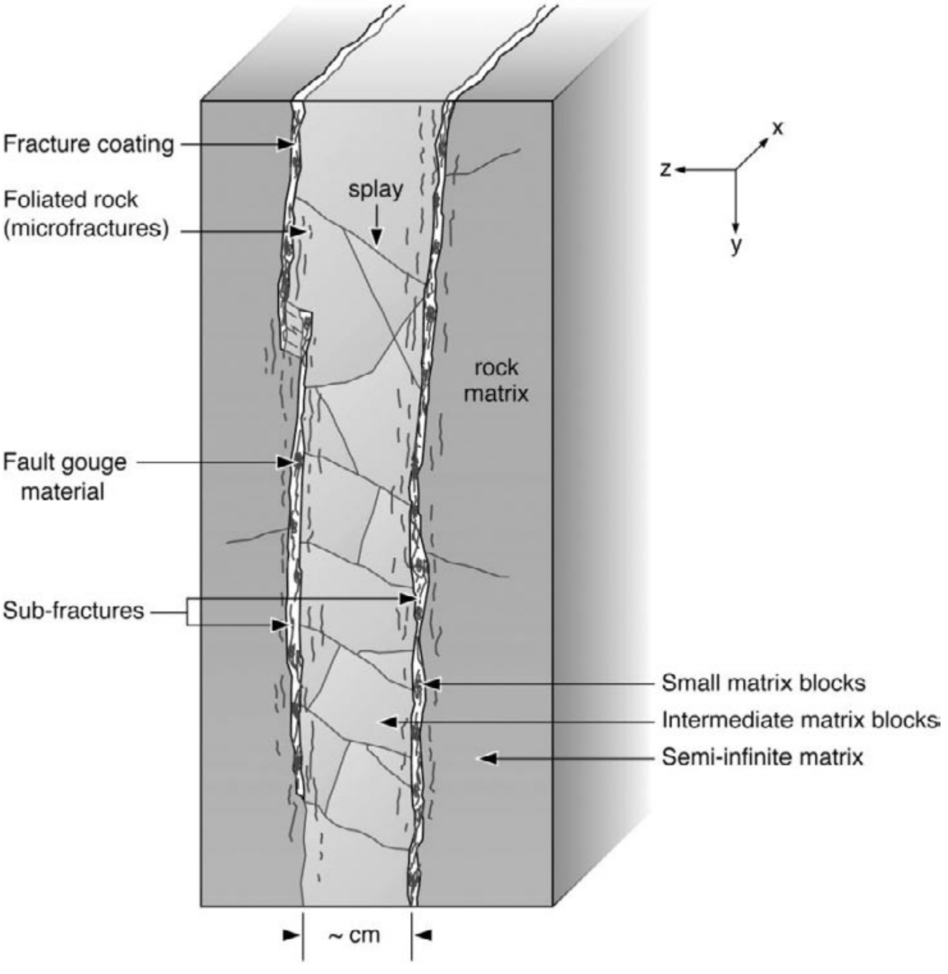

Figure 3-8. Structure of a complex fracture or master fault used by the JNC-LBNL team (adapted from /Mazurek and Jacob, 2002/).

parameter. Diffusion and sorption into the materials surrounding the sub-fractures are conceptualized as occurring in three matrix-block populations with different characteristic sizes: small (gouge material infilling the sub-fractures), intermediate (matrix blocks within the ladder structure), and large (semi-infinite or finite rock matrix outside the ladder structure). Each population was assigned its own porosity, effective diffusivity and sorption strength. Transport was calculated with the particle-tracking code THEMMB /Tsang and Tsang, 2001/, with analytical solutions used for diffusion and sorption.

3.8.2 Results and discussion

Model parameters that are not well constrained by available data were inferred from calibration to the breakthrough curves from the STT-1b tracer test. Good agreement was obtained for the non-sorbing tracers (HTO and I) by varying the heterogeneity of the fracture-transmissivity distribution, the fracture porosity, the relative proportion of small matrix blocks (gouge), and the fracture structure parameter α. Reasonable matches to the breakthrough behaviour for sorbing tracers (Sr, Co, and Tc) were obtained by increasing their sorption strength in the gouge material.

Preliminary results show that for performance assessment boundary conditions, the time required to traverse 10 m across the model is less than one month in the absence of any diffusion or sorption effects (transport solely by advection through the fracture network) and ranges from five months to 16,000 years for tracers with different sorption strengths, indicating that diffusion and sorption significantly retard tracer transport. Sensitivity studies illustrate how tracer breakthrough curves can develop double-humped shapes as a result of fracture-zone flow partitioning among large and small sub-fractures.

The new approach has been demonstrated to be feasible, to produce reasonable results and to include sufficient physics to account for structure within a complex fracture.

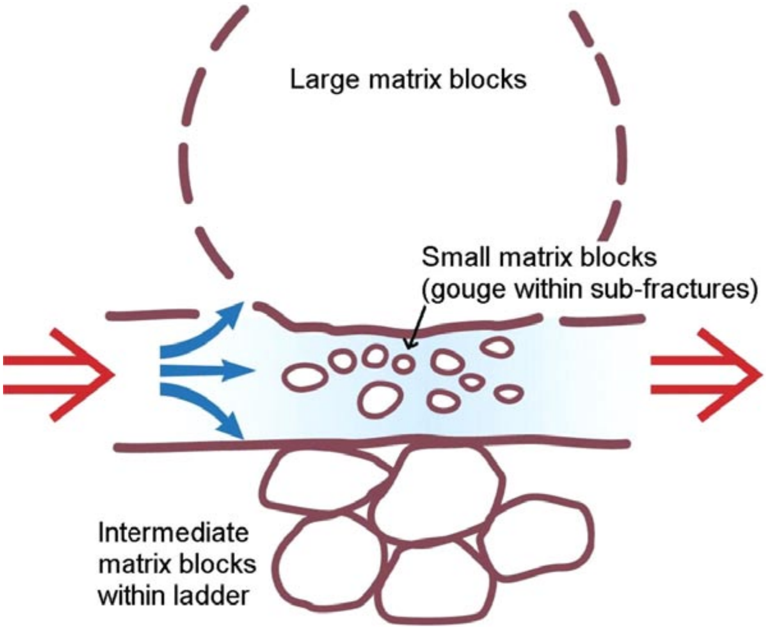

Figure 3-9. *Schematic representation of the three populations of matrix blocks used by the JNC-LBNL team /Doughty and Uchida, 2004/.*

A relevant question is how reliable parameters obtained from the Task 6A calibration are for simulating PA behaviour. Two factors come into play. The first is the large difference between the time scales of the STT-1b tracer test (4 hours to 40 days) and performance assessment tracer arrival times (up to 10,000 years). The second is the effect of fracture plane heterogeneity and the different flow paths activated by the tracer-test and PA boundary conditions.

The transmissivity spatial variation gives rise to flow channelling effects, which affect the so-called "effective flow wetted surface (FWS)" that is an important factor in certain calculational models simulating solute transport retardation due to diffusion and sorption. The relationship between FWS determined from short-term tracer tests and appropriate FWS to be used for long term PA is yet to be carefully evaluated. There is a good chance that FWS for PA may be more simply determined: because of potential "diffusion-saturation" of smaller heterogeneity features, their effect becomes a simple retardation factor for long times. The present method presents a useful approach for studying the relationship.

The JNC-LBLN team emphasise that gouge plays an important role in in-situ tracer experiments. If it is omitted then it is necessary to invoke unrealistically large matrix diffusivities or very large flow wetted surface or K_ds to explain enhanced retardation. A further important aspect of gouge is that it can provide access to the matrix in parts of the feature where there is little or no flow.

3.8.3 Review

The modelling approach used by the JNC-LBNL team encompasses both the complexity of the Feature A geometry and the complexity of diffusion/sorption into matrix zones in a manner that both reasonably honours the SC quantitative and qualitative information and can be used for PA calculations. It is particularly commendable that information on the ladder structure has been incorporated into the modelling. It would be good to further develop the model. Indeed this is currently underway, in particular to include fracture coating layers.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** The JNC-LBNL achieves a practical balance between SC complexity and PA simplicity that could usefully be taken further forward in the future.
2. **Determine constraining power of tracer and flow tests for PA:** The division of matrix zones into three populations emphasises that only the small blocks (gouge material infilling the sub-fractures) and possibly the intermediate blocks (matrix blocks within the ladder structure) are constrained by tracer tests, whereas PA calculations are dominated by the rock matrix outside the ladder structure. The effective flow wetted surface derived from short-term tracer tests may not be directly transferable to PA time scales.
3. **Support design of SC programmes for PA:** The JNC-LBNL model could act as a test bed for examining the relationship between SC data and PA parameters, for example the effective flow wetted surface under SC and PA conditions.
4. **Improve understanding using SC models:** The model provides a potential test bed for exploring the flow-wetted surface under SC conditions.

3.9 Posiva-VTT

The Posiva modelling team from VTT Processes used a PA stream tube approach, in which flow paths are represented by streamlines /Poteri, 2004/. The philosophy of using a PA model for tracer test analysis is as follows. It is recognised that the handling of the flow field is quite simplistic. However, the key parameter is the flow wetted surface per unit flow rate, which provides the hydrological control for interaction processes along the flow path. In many cases this parameter needs to be resolved through modelling but for radially converging tracer tests in a single fracture it can be robustly estimated from the flow rate through the injection borehole and the diameter of the borehole.

3.9.1 Approach

In Tasks 6A and 6B a single channel of aperture 2 mm, width 25 mm and length 5.03 m was used, while for the 2 m wide line source in Task 6B2 several parallel transport channels with varying flow rates were used.

The modelling takes into account three main processes: advection, matrix diffusion and sorption both on the fracture walls and in the matrix. Sorption, pore diffusivity and porosity properties are taken from the data given in the task specification. The geometry of the channel was modified to calibrate the modelled breakthrough against the measured outcome of the STT-1b test.

Matrix diffusion can take place in different geological units containing immobile pore water. Three different immobile pore spaces are considered: stagnant pools of the flow field, fault gouge and rock matrix (Figure 3-10). The basis of the model calibration was the measured breakthrough curves of ^{131}I, ^{85}Sr and ^{58}Co in the STT-1b test.

It should be noted that the single channel model always eventually gives 100% recovery. However, the STT-1b test does not show 100% recovery for all tracers.

The transport modelling approach is based on an analytical solution. In addition, matrix diffusion was modelled as a one-dimensional random walk process, and this approach was verified against an analytical solution for the case of an infinite matrix.

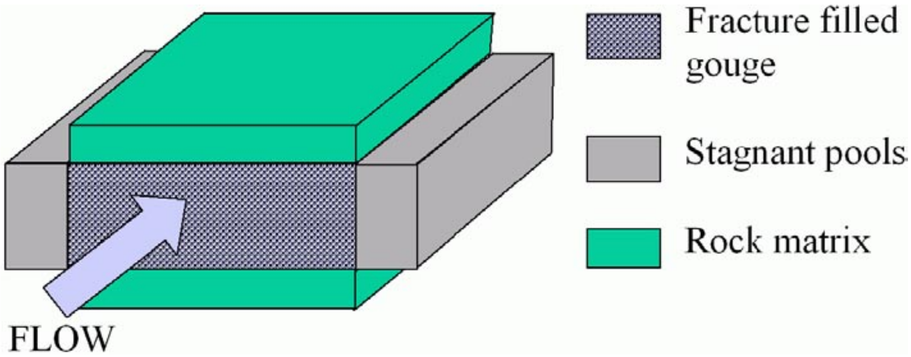

***Figure 3-10.** POSIVA-VTT conceptualisation of the immobile pore spaces and transport channel /Poteri, 2004/.*

3.9.2 Results and discussion

The Tasks 6A and 6B simulations show that retardation over the time scales of tracer experiments and PA may be dominated by different geological units. On the experimental time scale tracers can occupy the rather small capacity pore spaces, in particular fault gouge and stagnant pools. Also, the altered rim zone falls into this category, although this was not analysed in the present study.

The flow rate distribution applied in Task 6B2 is based on the flow rates measured in the five different boreholes intersecting Feature A. Naturally, this gives quite a coarse picture of the flow rate distribution and gives rise to peaky tracer discharge in the modelling results. In particular, the retention due to matrix diffusion is quite sensitive to the flow rate and this further enhances the differences in the retention potential of the different transport channels. This is reflected in the modelling results as a wider spread of the breakthrough curve. The first breakthrough takes place earlier than in the Task 6B and the tail is also longer.

3.9.3 Review

The POVIVA-VTT team has approached the study from a PA perspective although the PA model was modified to include matrix diffusion in stagnant pools and fault gouge in order to accommodate short-term diffusion and sorption effects occurring on an experimental time scale.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** A PA model can be used for both experimental and PA time scales provided that matrix diffusion into small capacity high diffusivity pore spaces (e.g. fault gouge, stagnant pools, altered rim zone) are included.
2. **Determine constraining power of tracer and flow tests for PA:** Short-term tracer tests do not significantly constrain the matrix parameters required for PA models.
3. **Support design of SC programmes for PA:** Site characterisation programmes should include direct measurements of the transport properties of the relevant matrix zones.
4. **Improve understanding using SC models:** The PA model could be fitted to the results of more complex models to provide effective parameters, thereby facilitating intercomparison and understanding.

3.10 SKB-CFE-SF

This section describes the work of the SKB modelling team from Computer-aided Fluid Engineering AB (CFE) and SF GeoLogic AB (SF) /Svensson and Follin, 2004/.

3.10.1 Approach

The SKB-CFE-SF conceptual model of exchange processes in Feature A is shown in Figure 3-11. The model assumes that there is one major flow channel, providing perhaps more than 90% of the total flow, and a number of secondary flow channels with much weaker flows (marked C in Figure 3-11). These secondary channels and possible cavities with circulation (D) give advective exchange with more or less stagnant water. It is important to note that the secondary channels may be very effective for retarding a tracer, both because they have a much lower velocity but also because they expose the tracer to larger volumes of truly stagnant water. Hence the "diffusive interface" can be significantly enlarged.

The main flow channel may be connected to other flow channels within the fracture (marked E) or to the three-dimensional fracture network, F. The influence of these may not be very significant if the pressure gradient is aligned with the main flow channel and everything is at steady state. Most interpretations of tracer transport and retardation assume steady-state flow conditions and this may be correct for an experiment with a pumped borehole as the local pressure gradients are determined by the pumping. For natural conditions (and long time scales) this assumption may however be questioned. It is easy to find transient processes on a wide range of time scales that can generate fluctuations (tidal effects, sea level variations, seasonal variations in precipitation, etc). It is unlikely that these will give rise to a perfectly uniform variation in pressure; instead one can expect time-dependent pressure gradients and hence flow to develop.

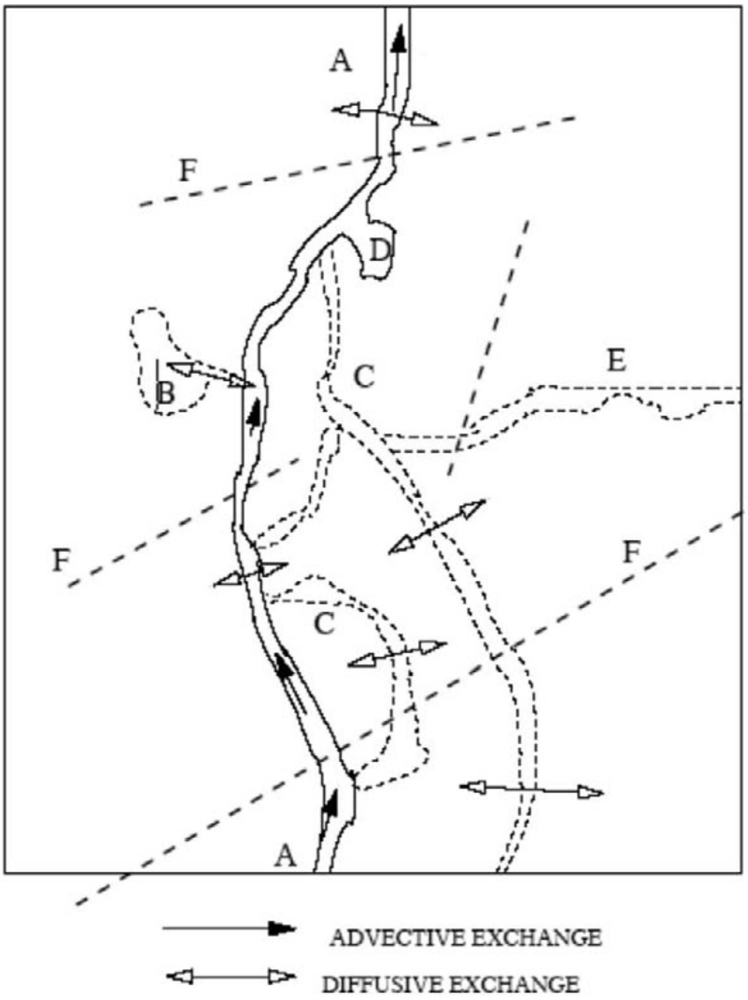

Figure 3-11. *SKB-CFE-SF conceptual view of exchange processes in a fracture plane: A. main flow channel; B. stagnant pool exchanging mass by diffusion only (dead-end volume); C. secondary flow channel; D. pool of water with advective exchange. E. flow channel which may be activated due to a transverse pressure pulse; F. crossing fracture that may provide a flow channel and connect the main flow channel to the thee-dimensional fracture network /Svensson and Follin, 2004/.*

It is argued that it may be important to consider transient effects when long-term transport under natural conditions is studied. In Figure 3-11, the crossing fractures (F) and the connected channel (E) may be activated and displace a tracer cloud significantly in the transverse direction. Also minor displacements from the main channel may be important as a small advective transport is often more effective than a purely diffusive exchange.

The model has been implemented in the finite-volume code DarcyTools /Svensson et al. 2003/ with processes occurring on a length scale less than the cell size using a sub grid model based on fractal scaling laws and multi-rate equations, FRAME. FRAME assumes that immobile zones can be represented by a set of boxes, each with its own length scale, volume and effective diffusion coefficient. Supporting research has been carried out to investigate how to parameterise sub-grid dispersion within FRAME /Svensson, 2004/.

3.10.2 Results and discussion

Simulations have been carried out for Tasks 6A, 6B and 6B2. Verification and validation studies indicate that the simulation model gives plausible results for weakly sorbing and non-sorbing tracers. For strongly sorbing tracers the results are more uncertain.

The role of near stagnant water in the fracture plane and the possible effects of transients have been considered. A simple generic test case showed that transient pulses might displace a tracer and hence affect the breakthrough curve.

This is the first study where DarcyTools has been used for tracer transport and retention studies. The strong and weak points of the model are listed below.

Strong points

- Fracture specification: It is possible to base a simulation on a detailed description of the fracture properties (porosity, FWS, conductivity, etc). Multiple pathways can be accounted for by the fracture network and property variations within the fracture zones.
- Multi-rate diffusion model: It is an advantage to be able to consider “diffusion volumes” with a wide range of capacities and exchange rates. For the present task the same specification of immobile zones has been used for the 1D experimental time scale, as for the 3D natural flow case.
- Numerically efficiency: For all simulations presented 100,000 particles were used in the simulations.

Weak points

- The current model cannot take detailed information about mineralogy and matrix properties into account, although in principle it could be extended to take account of such detailed information.
- For strongly sorbing tracers, it is possible that chemical reactions are more important than diffusive exchange. As the model is focused on diffusion, it may not be easy to accommodate these reactions.

3.10.3 Review

DarcyTools/FRAME is essentially a SC modelling tool although the treatment of sub-grid diffusive processes uses effective parameters that are not directly related to experimental data. Some of the more transient phenomena are not relevant to PA time scales, and it would be useful to make this clear and to clarify the overall modelling philosophy. This study is the first application to transport and retention problems and thus inevitably it has not been possible to carry out such a comprehensive analysis of Tasks 6A, 6B and 6B2 as some of the other modelling teams with more mature codes. Nevertheless, the approach shows promise of being a flexible SC modelling tool for incorporating relevant transport and retention processes in an efficient manner. However, further development is required to enable reliable modelling, for example of strongly sorbing tracers.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** Not addressed.
2. **Determine constraining power of tracer and flow tests for PA:** Not addressed.
3. **Support design of SC programmes for PA:** Time-dependent flow processes could be important on PA time scales and may need to be considered as part of site characterisation programmes.
4. **Improve understanding using SC models:** The model has the potential to help improve the understanding of flow effects within features, e.g. the effects of transient flows, but further work is required to draw definite conclusions.

3.11 SKB-KTH-ChE

The SKB modelling team from the Department of Chemical Engineering and Technology (ChE) at the Royal Institute of Technology (KTH) in Stockholm have used a channel network model, implemented in the CHAN3D code, to gain insights into the harmonisation of SC and PA models /Crawford and Moreno, 2004/.

3.11.1 Approach

The channel network model assumes that fluid flow and solute transport takes place through a network of interconnected channels. Within an individual channel, the tracer is transported by advective flow and can diffuse into the surrounding rock matrix. In addition, the model includes sorption within the rock matrix and on the channel surfaces. Sorption and diffusion data were obtained from compiled laboratory experimental values and the modelling input data set (MIDS).

The simulations were made using the CHAN3D computer program /Gylling, 1997/, which is based in the channel network model of /Moreno and Neretnieks, 1993/. The model takes into account the uneven flow distribution observed in fractured rock and the stochastic nature of the hydraulic features in addition to matrix diffusion and sorption.

The flow paths are assumed to make up a network of flow channels in the rock and the model concept assumes that fluid flow and solute transport take place in a three-dimensional network of channels. The hydraulic properties of individual channels can be generated by including the effects of different lengths, hydraulic conductivities, and other properties of interest. Data can be obtained from borehole transmissivity measurements and observations of fracture widths /Gylling et al. 1998/.

Conceptually, the channel network model considers that there can be up to six interconnected channels at the point of fracture intersection. This is partially based upon the premise that when fracture planes intersect, preferential flow paths or channels in the plane of one fracture can interconnect both with channels in the other plane as well as the stream tube along the line of plane intersection. The interconnecting channels at a fracture intersection may appear similarly to that shown in Figure 3-12.

Although the geometry of intersecting channels may be randomly oriented within the rock, the channel network model considers a regular, rectangular grid of channels as shown in Figure 3-13.

Each member of the network is assigned a hydraulic conductance, and in the current work these were assumed to be log-normally distributed and not correlated in space. Conductances are the only entity needed to calculate the flow, if the pressure field is known. If the residence time for non-interacting solutes is to be calculated, then the volume of the channel members is also needed.

Owing to lack of data, the channel volume was estimated by assuming that the conductance of a channel is proportional to the cube of the channel aperture. The constant of proportionality was estimated from the flow porosity, which in turn was determined from the residence time distribution for conservative tracers. If sorption onto the fracture surface or diffusion into the matrix is to be included in the model, the flow-wetted surface area must also be included. Some properties of the rock are needed, such as rock matrix porosity, diffusivity, and sorption capacity for sorbing species.

The properties of individual channels may differ considerably if a large standard deviation is used for the log-normal conductance distribution. This leads to a sparse flow system where there will be a few channels with relatively large flow rates and some with almost no flow at all, which is similar to what is observed in fractured rock when hydraulic tests are carried out.

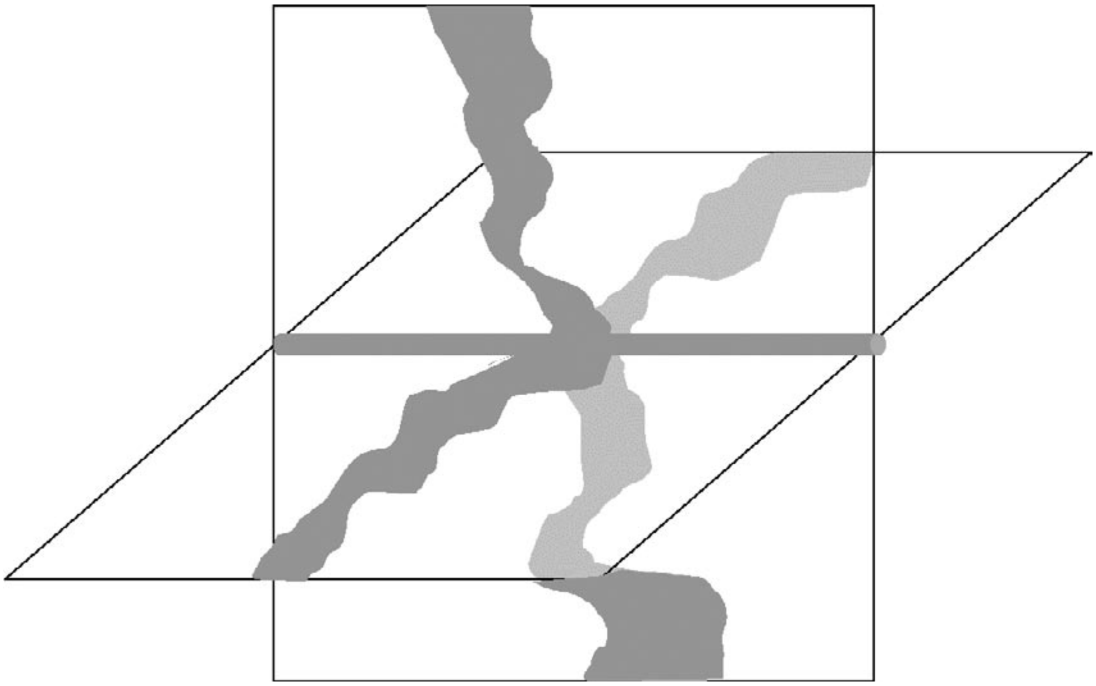

Figure 3-12. *Illustration of interconnected channels both within the fracture planes as well as at the line of fracture intersection /Crawford and Moreno, 2004/.*

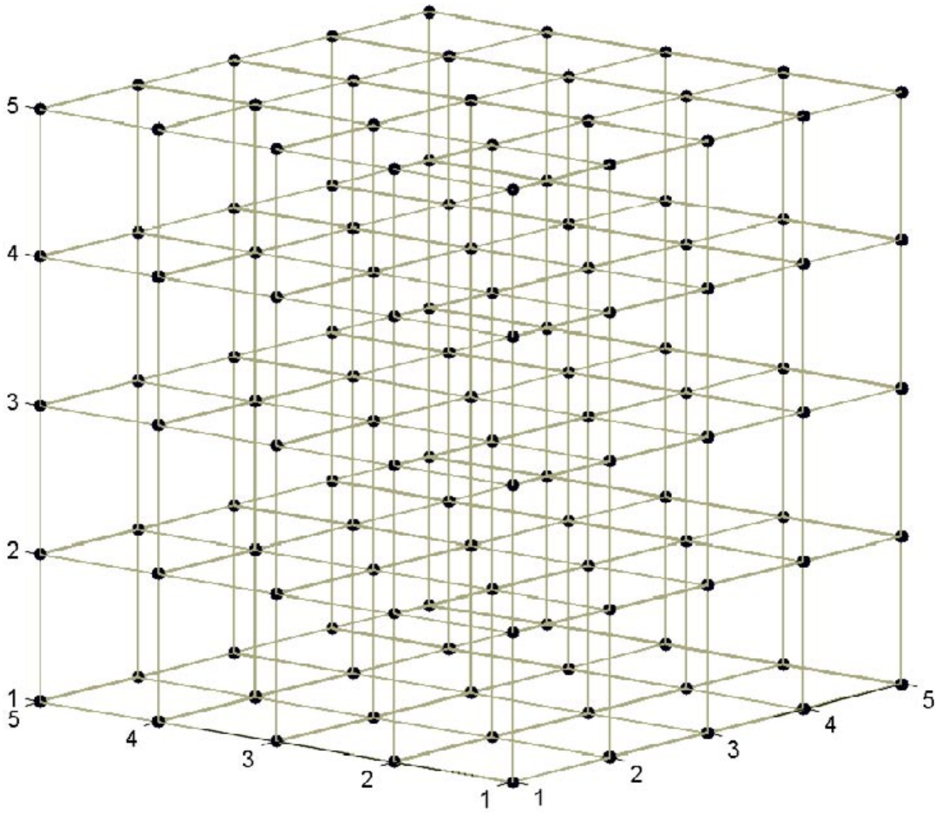

***Figure 3-13.** Schematic view of the channel network made up of interconnected mixing nodes. Each node is connected to six other nodes in a regular, rectangular grid arrangement /Crawford and Moreno, 2004/.*

Solute transport was simulated using a particle following technique /Robinson, 1984; Moreno et al. 1988/. Particles arriving at an intersection are distributed in the outlet channels with a probability proportional to their flow rates. The residence time of an individual particle along the whole path is determined as the sum of residence times in each channel that the particle has traversed. The residence time distribution is then obtained from the residence times of a multitude of individual particle runs. Hydrodynamic dispersion in the individual channels is considered to be negligible in comparison with the dispersion that arises from the varying transit times for particles taking alternate routes through the channel network.

3.11.2 Results and discussion

The recovery times for all sorbing tracers under the Task 6A hydraulic conditions are dominated by retardation due to surface sorption. For the high flow rates encountered in the flow structure, matrix interaction plays a very minor role for the estimated arrival times of 5% and 50% of the injected tracer mass. Only the trailing edge of the tracer pulse is influenced by matrix interaction processes.

Under the hydraulic conditions specified for Task 6B, surface sorption accounts for a much smaller proportion of the simulated tracer retardation and matrix interaction plays an overwhelming role for the transport time of the strongly sorbing tracer ^{241}Am. For the more weakly sorbing tracer ^{58}Co, surface sorption and matrix interaction may be equally important retardation mechanisms.

An attempt to reconcile the tracer breakthrough data was made by comparing results where 2D and 3D flow assumptions were used in the modelling. At present, it is not possible to conclude if the flow structure is 2D or 3D. However, there are several indications that a 3D flow structure is more probable. If a 2D flow structure is assumed, a mean fracture aperture of about 2 mm is required to match the flow rate pumped at the collection hole and the water residence time. Such large fracture apertures are not usually observed in the field. On the other hand, if it is assumed that the flow structure is 3D in nature, a more reasonable fracture aperture is obtained (0.07 mm). This fracture aperture is much closer to what would be expected, based upon previous experiences e.g., during the Stripa project /Birgersson et al. 1992/. Moreover, predictions of the sorbing tracer tests STT1 using only independent data /Neretnieks and Moreno, in press/ have shown a good agreement with the experimental breakthrough curves. Finally, the tracer travel times predicted using the 2D flow structure are much shorter than the experimental values for the sorbing tracer used in STT1 experiment.

The sorbing tracer ^{99}Tc has not been detected in the STT-1b experiment. However, the tracer should have been detectable in the recovery borehole within the time frame of the experiment according to the 2D simulation results. Breakthrough of tracer was predicted after 500 hours in the 2D simulations and after about 8,000 hours in the 3D simulations. The "no-show" of ^{99}Tc is consistent with the 3D simulations although not in any way conclusive.

The choice of injection node used in the simulations can have a small influence upon the results, although the differences are usually quite minor. The arbitrary choice of channel length used in the simulations appears to only have a minor influence on the consistency of the simulation results. The largest differences appear in very heterogeneous networks where there are only a few channels separating the injection and recovery nodes. Provided that there are at least 15–20 channels in the fastest route separating the injection node from the recovery node, the differences appear to be, for all practical purposes, negligible within the present context.

The simulation results made in connection with Task 6B2 show that the uncertainty concerning the Feature A transmissivity relative to the background transmissivity field has a very strong influence upon the tracer recovery times. This was not fully explored in the Task 6A and 6B simulations as only the two limiting flow scenarios were studied (i.e. purely 2D flow, and 3D flow with no increased Feature A transmissivity). Many of the qualitative observations made in the Task 6A and 6B studies were also noted for Task 6B2. In particular, it was found that the flow porosity could be varied over several orders of magnitude without affecting the breakthrough characteristics for strongly sorbing tracers. It was also found that matrix interaction played an overwhelmingly important role for tracer retardation and surface sorption processes had very little influence upon the tracer recovery times.

3.11.3 Review

The channel network model approach used by the SKB-KTH-ChE modelling team provides a useful alternative perspective on modelling flow heterogeneity for Feature A and the surrounding rock mass. It is noted that the concept of flow occurring in a network of channels is consistent with a range of observations in low permeability crystalline rocks /Abelin et al. 1985, 1990; Bourke, 1987; Moreno and Neretnieks, 1993/. However, CHAN3D essentially assumes the same distribution of cunductances for channels within fractures and along fracture intersections, which is a questionable assumption.

The team has used the model to explore questions related to the dimensionality of Feature A by examining the limiting cases of 2D and 3D flow. While the evidence is not conclusive, there are indications that flow is taking place in more than a single planar fracture, which is consistent with the site characterisation data /Winberg et al. 2000/. This matter can only be resolved by more detailed experimentation of the sub-structure of flow in Feature A.

The finding that the recovery times for all sorbing tracers under Task 6A hydraulic conditions are dominated by retardation due to surface sorption is consistent with the results of other modelling teams if surface sorption is considered to be due to a combination of fast processes near to channel surfaces.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** Until the geometric model for flow is understood more clearly it is difficult to make any definitive statements about the validity of simplifications for PA.
2. **Determine constraining power of tracer and flow tests for PA:** Tracer tests do not constrain the long-term matrix diffusion and sorption parameters that control transport on PA time scales.
3. **Support design of SC programmes for PA:** More in-depth studies are needed to understand the flow sub-structure of Feature A or related features.
4. **Improve understanding using SC models:** The channel network approach is potentially useful for understanding flow within Feature A, but further information on the channel characteristics is required.

3.12 SKB-KTH-TRUE

The SKB modelling team from the Department of Water Resources Engineering of the Royal Institute of Technology (KTH) in Stockholm used the Lagrangian Stochastic Advection and Retention (LaSAR) modelling approach /Cheng and Cvetkovic, 2004/ for Tasks 6A, 6B and 6B2. This approach is described in more detail in /Cvetkovic et al. 1999, 2000/. It has also been used to evaluate sorbing tracer tests within the TRUE-1 programme /Winberg et al. 2000/ and thus the team is designated SKB-KTH-TRUE.

3.12.1 Approach

Feature A is assumed to be a planar fracture with variable spatial apertures. The distribution of the apertures is approximated to be log-normal with an exponential correlation structure. The porosity is assumed to be constant.

The following mass transfer processes are accounted for in the modelling: advection, dispersion, sorption on fracture surface, and diffusion/sorption in the rock matrix (Figure 3-14).

The model is parameterised in terms of two flow-dependent parameters which influence diffusive mass transfer: the water residence time (τ) and the water residence time per unit half-aperture, β, which is a random quantity integrating the inverse of the velocity-weighted variable aperture along a flow path. The parameter β controls surface sorption and diffusion/sorption into the rock matrix, and takes into account the effect of flow heterogeneity on

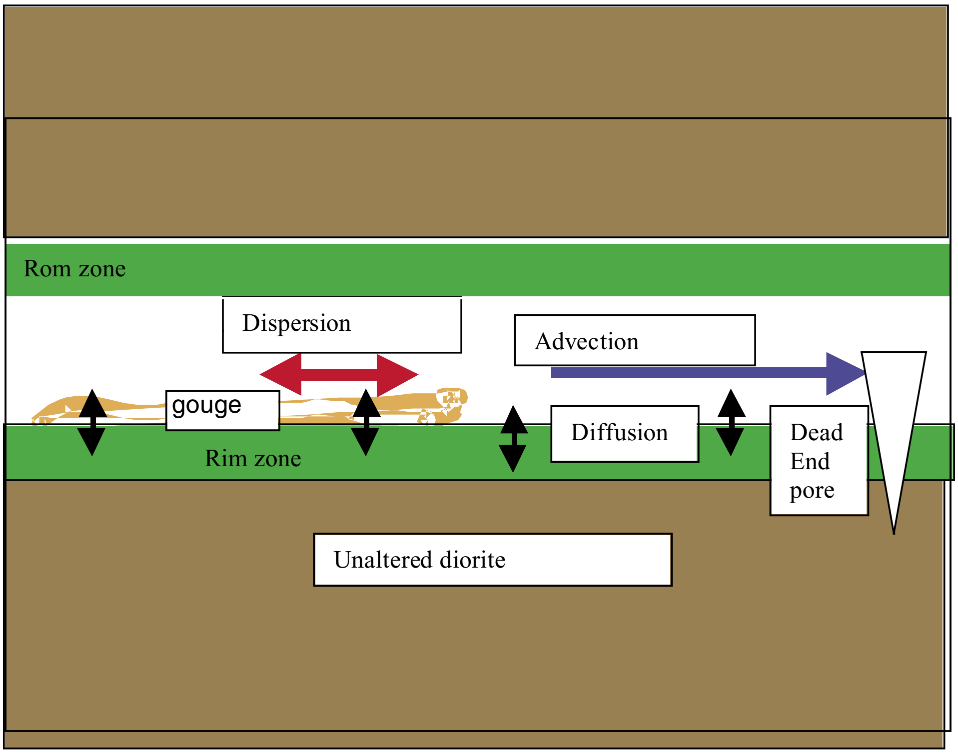

Figure 3-14. *SKB-TRUE conceptual model /Cheng and Cvetkovic, 2004/.*

the mass transfer reactions. A linear τ-β relationship inferred from the TRUE-1 evaluation /Cvetkovic et al. 2000/ was used in calculating the breakthrough curves (BTCs) in Tasks 6A and 6B. The distribution of τ was assumed to be inverse-Gaussian. The moments of τ calibrated in the TRUE-1 evaluation for STT-1b were also used in Tasks 6A and 6B.

In the modelling for Tasks 6A, 6B and 6B2, the best estimates of sorption and diffusion parameters from the TRUE-1 evaluation were used. In Task 6B, a second set of modelling results were also provided using an additional lower porosity value representative of the undisturbed rock matrix rather than the altered rim zone.

In Task 6B2, a second set of modelling results were provided using a porosity from the MIDS data set /Byegård et al. 2001/. The simulated τ, β data from Monte-Carlo simulations were used directly in the calculation of BTCs in Task 6B2.

3.12.2 Results and discussion

In Task 6A, the BTCs and the times for 5%, 50% and 95% mass recovery are comparable for both the experimental injection and the Dirac pulse injection. This could imply that, as long as the injection duration is not so long, the injection history has relatively small influences on the retention of the tracers.

In Task 6B, the influences of porosity on tracer retention are apparent. For Dirac injection, the ratios between the respective mass recovery times for the two porosities are always larger than the ratio of the porosity itself (which is 2). This indicates that the influences of the porosity are non-linear and are larger for larger porosities.

The modelling results of Tasks 6B and 6B2 show that the parameter β has a strong influence on retention and transport, and therefore on the breakthrough curves of the tracers.

There are differences between the BTCs of the same tracer in Tasks 6B and 6B2, when using the same porosity and the same value of sorption coefficient. The retention of the tracer is stronger in Task 6B2 than in Task 6B. The reason for the difference is that, in Task 6B2, the values of β are obtained from Monte-Carlo simulations while in Task 6B, the values of β are assumed to be linearly related to the water residence time τ.

In summary, the LaSAR approach seems suitable both for evaluating the site characterisation results and in providing reasonable estimates for performance assessment modelling.

3.12.3 Review

The LaSAR approach used by the SKB-TRUE team straddles the SC and PA divide and thus provides a useful benchmark for Task 6. The approach is rather mathematically complex and would benefit from some schematic diagrams illustrating the concepts and parameter definitions.

For the systems and parameters considered in this study, the implications for the Task 6 objectives 1–4 (Section 1.5) include:

1. **Assess simplifications for PA:** The LaSAR approach appears to be a suitable PA tool, with input derived from SC models and data. It thus provides a methodology for transforming SC models and data into PA models in a consistent manner.
2. **Determine constraining power of tracer and flow tests for PA:** The results confirm the findings of other teams that short-term tracer tests do not significantly constrain the matrix parameters required for PA models.
3. **Support design of SC programmes for PA:** The LaSAR approach provides a bridge between SC programmes and PA.
4. **Improve understanding using SC models:** Not directly applicable to this study.

4 Overall evaluation and review

This section presents an overall evaluation and review of the modelling team approaches and results for Tasks 6A, 6B and 6B2.

4.1 Modelling team approaches

The wide diversity of approaches discussed in Section 3 is a testament to the value of the Äspö Modelling Task Force in providing alternative perspectives from which to develop an understanding of the structures and processes that govern the transport of solutes in low permeability fractured crystalline rocks. This section presents an overall review and evaluation of the approaches adopted by the modelling teams.

4.1.1 Flow geometry

As regards the flow geometry, most teams assumed that Feature A was a single fracture. However, a range of flow complexities were considered within this assumption as follows:

- The simplest approach was to assume an effective single channel connecting the injection and extraction boreholes in a straight line. This can be justified on the basis of Occam's razor or in Einstein's words "everything should be made as simple as possible but not simpler", and is the natural choice for a PA model in the absence of evidence to the contrary.
- At the next level of complexity, a 2D spatially varying flow field was derived from the results of modelling heterogeneous transmissivity distributions based on hydraulic test data from the five boreholes intersecting Feature A.
- A complementary approach to in-fracture heterogeneity was provided by channel network models based on generic evidence that flow tends to occur in one-dimensional channels.

The spatially varying flow field and channel network models would benefit from more extensive and detailed characterisation data.

The JNC-LBNL team explored some consequences of Feature A having a sub-structure with a more three-dimensional flow geometry, for which there is some qualitative evidence from the site characterisation studies /Winberg et al. 2000; Mazurek and Jacob, 2002/. Also, the SKB-KTH-ChE team explored the coupling of flow within Feature A with 3D flow in the surrounding rock. It is particularly interesting that the SKB-KTH-ChE team found fracture apertures to be more realistic for their 3D network compared to their 2D network. Approaches that account for the three-dimensional sub-structure of features and their coupling to the surrounding rock should be further developed in future.

From the perspective of flow connectivity, it is seen that all groups modelled Feature A as well connected. The channel network models and the stochastic transmissivity models have the capability to make the connectivity of channels within Feature A poorly connected. However, the parameters chosen within this exercise result in a well-connected channel structure, based on the hydraulic evidence from the five boreholes that intercept Feature A.

Outside Feature A, only the SKB-KTH-ChE 3D model assumes that there is any flow connectivity with rock, thereby allowing more dilution in the collection borehole. While this general lack of connectivity outside Feature A may be an adequate assumption for the boundary conditions and timescales of tracer tests, it is unlikely to hold true for the boundary conditions and timescales of relevance to repository safety.

Overall, with some notable exceptions, the flow geometries adopted by the modelling teams lacked the complexity and realism that might be expected for site characterisation models at the scale of Feature A. In particular, it is an over-simplification for SC modelling purposes to assume that Feature A is a planar fracture with no structure in the third dimension and that it is decoupled from the surrounding rock.

The fact that such a range of flow geometries could be postulated for Feature A by highly competent groups based on the same state-of-the-art site characterisation data, emphasises that there still remains significant uncertainty in characterising and modelling flowing features in sparsely fractured rock. In particular, channelling and the β parameter are still not well constrained despite extensive characterisation and interpretation. This lack of consensus on how to model flow in sparsely fractured rock is an unresolved issue for solute migration modelling in relation to site characterisation, performance assessment and the safety case.

The only way to reduce this uncertainty is further detailed experimentation on the scale of Feature A or related structures. However, uncertainty can never be reduced to zero, and the most important question is whether it has been reduced sufficiently with reference to the development of a safety case for a particular system. In this context, the Task 6 approach of applying multiple conceptual models consistent with site characterisation data can provide bounds on the impact of uncertainty on repository performance.

4.1.2 Dispersion

Dispersion represents hydrodynamic mixing processes on a smaller scale than is included explicitly in a model. Thus the treatment of dispersion can be expected to be different for different model implementations. In the opinion of the reviewers the representations of dispersion by the modelling teams were generally appropriate for the problem at hand. However, it would have been relevant to have made an independent estimate of the size of dispersion due to advective mixing between slow and fast channels /Becker and Shapiro, 2000, 2003/ in order to check that this is not the dominant mechanism under the conditions considered.

4.1.3 Pore space interactions

/Mazurek and Jacob, 2002/ and /Jacob, 2004/ have documented geological evidence for the occurrence of pore space diffusion in the TRUE-1 block and at other locations, which provides a sound basis for the inclusion of this process by the modelling teams.

Also, many analyses have deduced the action of matrix diffusion based on inverse power law tailing of tracer breakthrough curves. However, large effective values of diffusivity derived from such tailing can under some circumstances be due to hydrodynamic dispersion due to tracer advection between slow and fast channels /Becker and Shapiro, 2000, 2003/. Thus, as noted in the previous section, it would have been useful to have documented the reasons for assuming that the primary mechanism under the conditions of Tasks 6A, 6B and 6B2 is diffusion rather than dispersion.

In principle, the diversity of approaches for treating the interaction of solutes with pore spaces outside the main flow regime has been less wide ranging than for flow, demonstrating a convergence of view. In practice the differences have been primarily related to model implementation rather than to underlying conceptual uncertainty. Thus all groups have included interaction with at least two pore spaces, at least one of which occurs on the time scale of tracer experiments and at least one of which occurs on PA time scales. The range of implementation of these concepts within the present exercise included:

- Explicit modelling of diffusion into matrix pores and linear equilibrium sorption onto pore surfaces for one or more of: stagnant pools; gouge/breccia; fracture coating; altered rim; mylonite; and intact rock.
- Explicit treatment of equilibrium sorption onto fracture surfaces, some of which could be attributed to fast diffusion and sorption into near-fracture pore spaces such as stagnant pools and gouge/breccia.
- Diffusion and sorption into effective zones representing the range of diffusivities and diffusive/sorptive capacities of pore spaces. It can be argued that this concept is self-consistent so there is no need to alter included processes and/or parameters when moving from SC to PA time scales.
- Advective coupling with slow moving or transient flowing regions within the flowing pathway.

Whatever the precise implementation of these concepts, there was general agreement that tracer experiments do not constrain interactions with pore spaces on PA time scales, and this is a major conclusion of Tasks 6A, 6B and 6B2. Indeed, the paradigm shift to the general use of models with multiple pore spaces can be seen as one of the key achievements of the Äspö Modelling Task Force.

Diffusion into gouge plays a particularly important role in in-situ tracer experiments. If it is omitted then it is necessary to invoke unrealistically large matrix diffusivities or very large flow wetted surface or K_ds to explain enhanced retardation. Finally, gouge can provide access to the matrix in parts of the feature where there is little or no flow.

This review has not been able to make any detailed checks on the numerical accuracy of the codes. However, it is noted that, where finite-element and finite-differences methods are used for diffusion into the matrix, it is necessary to use a reasonably fine discretisation in order to model the concentration gradient with sufficient accuracy.

To take these matters further it might be worthwhile to decouple diffusion and sorption from flow and to consider a further exercise specifically aimed at validating models of diffusion and sorption from stationary water next to fracture surfaces into the surrounding rock. Such an exercise might uncover some problems with the use of the linear equilibrium sorption assumption. For example it is plausible that in some circumstances sorption kinetics need to be included on the time scale of field experiments /Hodgkinson and Lever, 1983/. Also, understanding of potential effects such as pore plugging may be enhanced through the use of coupled reactive transport models including a range of relevant chemical reactions.

As noted by /Jacob, 2004/ there are a number of other open issues and unresolved problems concerning diffusion and sorption into stagnant pore spaces, including the limited extent of the porous matrix for diffusion to values of the order of centimetres or decimetres, which can have a profound effect on radionuclide transport predictions. The issues raised by /Jacob, 2004/ deserve continued consideration in future research programmes.

4.1.4 Inverse modelling methodology

A further perspective on the work of the different modelling teams relates to the type of methodology used to extract information from the test data. In general the following methodologies have been used:

- Deterministic best fit of relevant model parameters to test data.
- Deterministic best fit of relevant model parameters to test data together with sensitivity and uncertainty analysis to determine reasonable parameter ranges.
- Probabilistic sensitivity analysis.

For providing input to PA it is appropriate to use either the second or third approach in the above list in order to propagate appropriate uncertainties. However, if parameters are represented by uncorrelated distributions, when in reality they should be correlated, then inconsistent combinations of parameters would arise and the overall uncertainty would be over-estimated. A practical solution to this problem has been advocated by the ANDRA-Golder team in terms of the following general probabilistic sensitivity analysis methodology.

1. Use as much general data as possible to develop given (prior) distributions for parameters chosen to be as uncorrelated as possible.
2. Use the given parameter distributions as input data for SC modelling. Only realisations that produce an acceptable match to field test data (e.g. combinations of tracer tests, pump tests, laboratory analyses of chemical properties etc) sets should be propagated to the PA modelling.
3. Carry out PA modelling for the specific combinations of parameter values that passed all tests against field data (the constrained coupled parameter distributions).

Possibly there should also be a stage between 2 and 3 where an effort is made to understand the alternative conceptual models embedded within the accepted realisations, for example using cluster analysis, so that these can be propagated individually.

A further way to deal with the issue of correlations is to carry out the analysis in terms of theoretically-motivated parameter groups rather than for the individual model parameters. For example, the JNC-Golder team found that for Task 6A the physical parameters of the solute transport model were not well constrained, but parameter groups such as the mobile/immobile volume ratio were constrained.

It is reassuring that the conclusion about the lack of constraining power of tracer tests for PA retardation parameters did not depend on the precise inverse modelling methodology used.

Indeed the above conclusion can be generalised to the statement that short-term experiments cannot constrain long-term behaviour. Thus if the Task Force would like to investigate slow processes contributing to long-term behaviour it would be necessary to analyse long-term information for example from natural analogues or palaeohydrogeological investigations.

4.2 Modelling team results

This section presents an overview of the collective experience of the modelling teams by attempting to draw out relevant achievements and unresolved issues from the ensemble of results. It is emphasised that it is not meant to be a detailed inter-comparison of the models as presented by /Elert, 2003/, but rather is intended to provide a complementary perspective to the review of individual models presented in Section 3. However in the interests of deepening understanding, an effort is made to explain the underlying reasons for the spread of results.

In the following discussion, the results are illustrated by the breakthrough time for the recovery of 50% (t50) and the maximum release rate for a Dirac pulse input for each of the tracers ^{131}I, ^{85}Sr, ^{58}Co, ^{99m}Tc and ^{241}Am.

4.2.1 Task 6A

Figures 4-1 and 4-2 show a selection of deterministic results for the 50% breakthrough time and maximum release rate for a Dirac pulse in Task 6A. These figures are based on /Elert, 2003/, but with updated results for the KTH-ChE team /Crawford, 2004/.

As shown in Figures 4-1 and 4-2, in Task 6A there is a reasonable consensus for the non-sorbing tracer, I. This indicates that all models are flexible enough to be calibrated to the flow rate and dispersivity of the tracer test. However, for the sorbing tracers, with the possible exception of Sr, there are significant differences in results as discussed in turn below.

It should be noted that the maximum release rate results for the KTH-ChE team shown in Figure 4-2 represent the mean of the maxima for a number of realisations. However, the standard deviations for these results are of a similar magnitude to the mean values, which implies that the KTH-ChE models are capable of generating realisations that are consistent with the tracer test data.

A similar result holds for the other stochastic approaches, in particular the ANDRA-Golder /Holmén and Forsman, 2004/ and JNC-Golder /Dershowitz et al. 2004/ analyses discussed in Sections 3.3 and 3.7. These studies also found stochastic realisations that are consistent with the tracer data. More importantly, they took the analysis one step further and assessed the degree to which transport parameters are constrained by the requirement that they are consistent with the tracer data.

In particular, an important conclusion from the JNC-Golder study /Dershowitz et al. 2004/ is that parameter groups are constrained as shown in Table 4-1. The parameter groups shown in Table 4-1 are defined as follows: a_r = 2/(aperture+2×Dmax); F = 2×travel time/aperture; k = porosity×$(D_{eff}\times R_{matrix})^{1/2}$; Volume Ratio = (Matrix Volume/Flowing Volume)×travel time×Retardation = ((2×Dmax+e)×n/e)×t×R. Table 4-1 provides a clear quantitative demonstration that the Volume Ratio is tightly constrained, while k and the F (or β)) factor are poorly constrained by the tracer data.

It is relevant to try and understand the primary cause of the spread of results for sorbing tracers shown in Figures 4-1 and 4-2. The close agreement for the non-sorbing iodine results among the deterministic analyses means that the flow rate and dispersivity are not the primary cause, even though, as discussed in Section 4.1.1, there is considerable uncertainty in the conceptual and mathematical models of flow in sparsely fractured rock. The two remaining possibilities are the sorption coefficients and the β parameter, as discussed below.

The values of t50 for sorbing tracers are expected to be approximately proportional to the sorption coefficients (e.g. see equations 4.1 and 4.2 below). It is thus encouraging that the values of t50 in Figure 4-1 increase in line with the characteristic strength of sorption coefficients from the weakly sorbing Sr to the strongly sorbing Am.

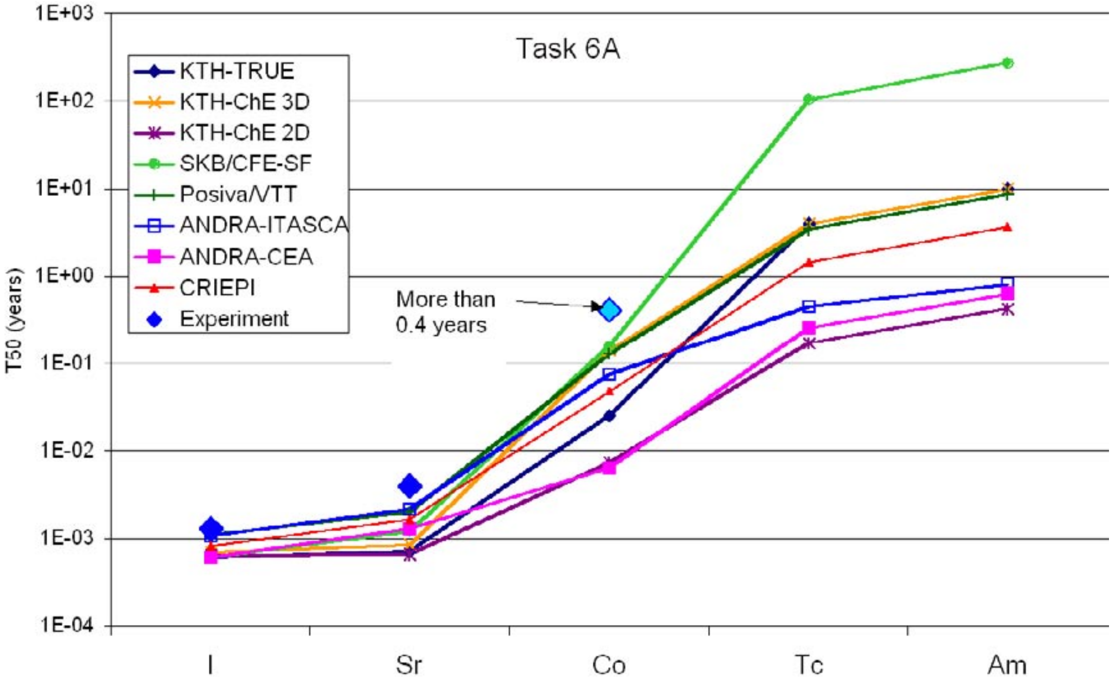

Figure 4-1. *Compendium of results for the 50% breakthrough time (y) for a Dirac pulse in Task 6A.*

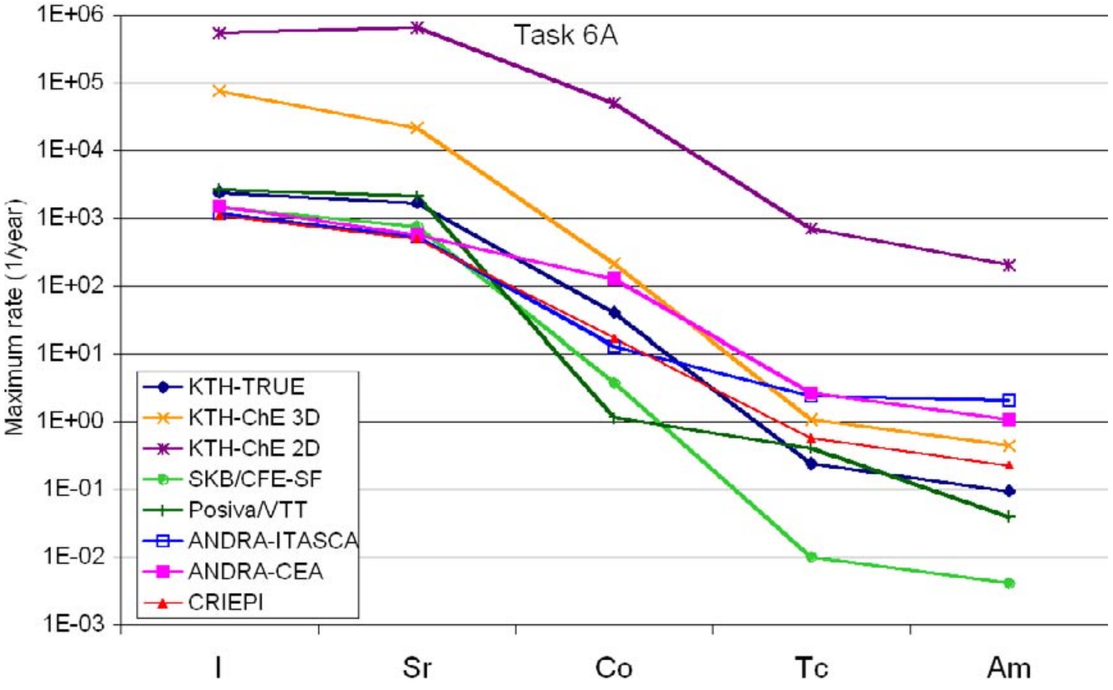

Figure 4-2. *Compendium of results for the maximum release rate (1/y) for a Dirac pulse in Task 6A.*

Table 4-1. Constraints on the range of values of parameter groups derived from the 10 simulations with the lowest error out of an ensemble of 1,500, for the JNC-Golder analysis /Dershowitz et al. 2004/.

Parameter group	a_r	F factor (or β)	k	k×F	k×F×t	Volume ratio
I-131 proportion of range	7.41%	27.41%	93.87%	14.00%	5.44%	0.45%
Sr-85 proportion of range	6.62%	72.52%	52.42%	12.42%	9.69%	0.16%
Co-58 proportion of range	16.09%	53.92%	39.37%	23.52%	18.28%	1.42%

It is noted from Figure 4-1 that the spread of t50 results also increases from Sr to Am. Thus it is interesting to see whether the variability of sorption coefficients used by the modelling teams increases with sorption strength from Sr to Am. This is addressed in Figure 4-3, which shows the ratio of maximum to minimum values of diffusion and sorption parameters used by the modelling groups. For the near-fracture materials (gouge and altered rim) it is seen that the spread of sorption parameters used does not increase from Sr to Am. It is in fact largest for Sr and approximately constant for Co, Tc and Am. Thus the spread of sorption coefficients used by the modelling teams is not the primary cause for the spread in t50 results.

To gain an understanding of these results it is useful to consider how t50 depends on the various parameters. While no universal formula is to hand, insight can be gained from formulae for the time of maximum discharge (t_{max}) presented in /Poteri, 2004/ for a single channel of constant width with surface sorption and diffusion into an infinite matrix. When surface sorption dominates,

$$t_{max} = t_w + \beta K_a , \qquad (4.1)$$

and when matrix diffusion dominates,

$$t_{max} = t_w + \beta^2 D_e \varepsilon R_p / 6, \qquad (4.2)$$

where t_w is the water transit time, $\beta = 2 WL/Q$ where W and L are the channel width and length, Q is the water flux, K_a is the surface sorption coefficient, De and ε are the matrix diffusivity and porosity, and $R_p = 1+\rho K_d/\varepsilon$ is the retardation coefficient in the matrix with ρ and K_d being the matrix density and equilibrium sorption coefficient.

It is important to note that the beta-factor (β) can be defined for a range of models used within Task 6 /Elert and Selroos, 2004/ in terms of the ratio of flow wetted surface to water flux and thus equations (4.1) and (4.2) can be expected to have a more general validity. However, there is no model-independent definition of β. This parameter group gives a measure of the surface area available for matrix interaction and the time constant for matrix interaction to occur. The beta-factor is an integrated quantity that monotonically increases along a flow path.

While t50 and t_{max} are not identical, they can be expected to have similar parametric behaviour. Thus for reasonably sorbed tracers it is expected that t50 will be proportional to the sorption coefficient, whether it is surface or matrix sorption, as discussed above. A key observation is that in these formulae the sorption coefficients are multiplied by β for surface sorption and β^2 for matrix sorption and thus differences in the β factors used by the modelling teams will result in the a spread of t50 values that increases with the strength of sorption.

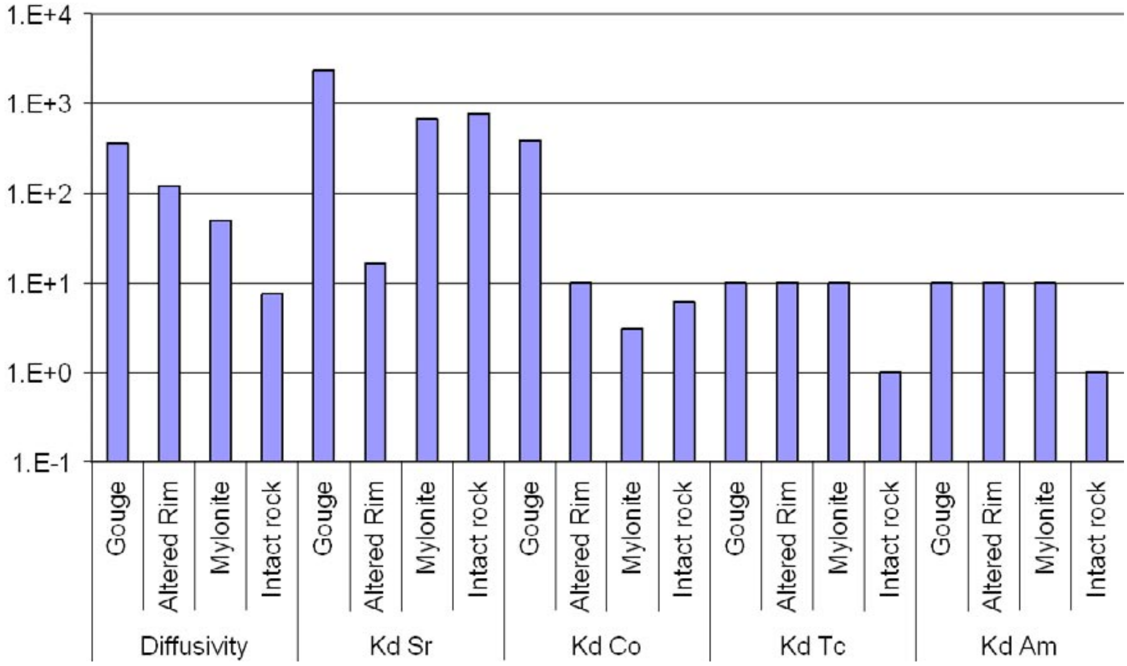

Figure 4-3. Ratio of the maximum to minimum values of diffusivity and Kd used by the modelling teams for gouge, altered rim, mylonite and intact rock /Elert, 2003/.

From (4.1) and (4.2) it can be seen that for surface sorption the slopes of the curves in Figure 4-1 from Sr to Am are proportional to β, while for matrix/diffusion/sorption they are proportional to $\beta^2 D_e \varepsilon$. In both cases, different values of β give rise to different slopes and hence to a spread in predictions of t50. Thus it is plausible that the range of values chosen for β by the different modelling groups is the primary cause of the differences between model predictions. Put another way, it appears that β is not highly constrained by the tracer tests.

It would therefore be interesting to compare the divergence of predictions for t50 with the corresponding divergence of β used by the different modelling teams. Unfortunately, β has not in general been specified by the modelling teams and so at present it is not possible to make such a comparison.

One possible way forward would be to make use of a single channel model with surface sorption and diffusion/sorption into the matrix to fit the t5, t50 and t95 values provided by the modelling teams in order to estimate effective values of β and other parameters. This would provide a way of summarising and understanding the results. In addition, it would aid understanding of the results if approximate formulae were derived for t50 (or t_{max} as a surrogate for t50) and for the maximum release rate for the case where solutes are affected simultaneously by surface sorption and diffusion/sorption.

In summary, the above evaluation points to the importance of the β factor in the interpretation of tracer tests. It would be useful to compile the effective values of β for the different modelling groups and to scrutinise their justification. If, as seems likely, there is insufficient evidence underpinning the choice of β, then further research may be required to improve this situation.

4.2.2 Task 6B

Figures 4-4 and 4-5 show the 50% breakthrough time and maximum release rate for a Dirac pulse for a selection of deterministic results for Task 6B divided by the Task 6A results. These figures are based on /Elert, 2003/, but with corrected t50 results and updated mean values for the stochastic KTH-ChE results /Crawford, 2004/. These graphs show that the models extrapolate differently to PA timescales. The spread in the 6B/6A results is not problematic in itself. It is simply a manifestation of residual uncertainty that is not sufficiently constrained by the tracer measurements and other site characterisation data. However, it is important to try and understand the differences between 6B/6A results so that the most important assumptions can be identified and the potential for further constraints on the system can be ascertained.

For the strongly sorbed elements (Tc, Am and to a lesser extent Co) transport is dominated by diffusion into immobile pore spaces, namely the gouge and altered rock for 6A, and the intact rock matrix for 6B. The 50% breakthrough time for 6B relative to 6A, as shown in Figure 4-4 is therefore expected from (4.2) to be:

$$t50\ [B]\ /\ t50\ [A] \approx 10^6\ (D_e\ \varepsilon\ R_p)\ [B]\ /\ (D_e\ \varepsilon\ R_p)\ [A], \qquad (4.3)$$

assuming that the flow geometry remains constant. In this formula, the value 10^6 is the square of the ratio of groundwater fluxes for the two cases, and $(D_e\ \varepsilon\ R_p)$ [A/B] means that effective values of these quantities of relevance to the timescales of Tasks 6A and 6B should be used. For example (4.3) is accurate to within 6% for the Posiva-VTT results for Tc and Am.

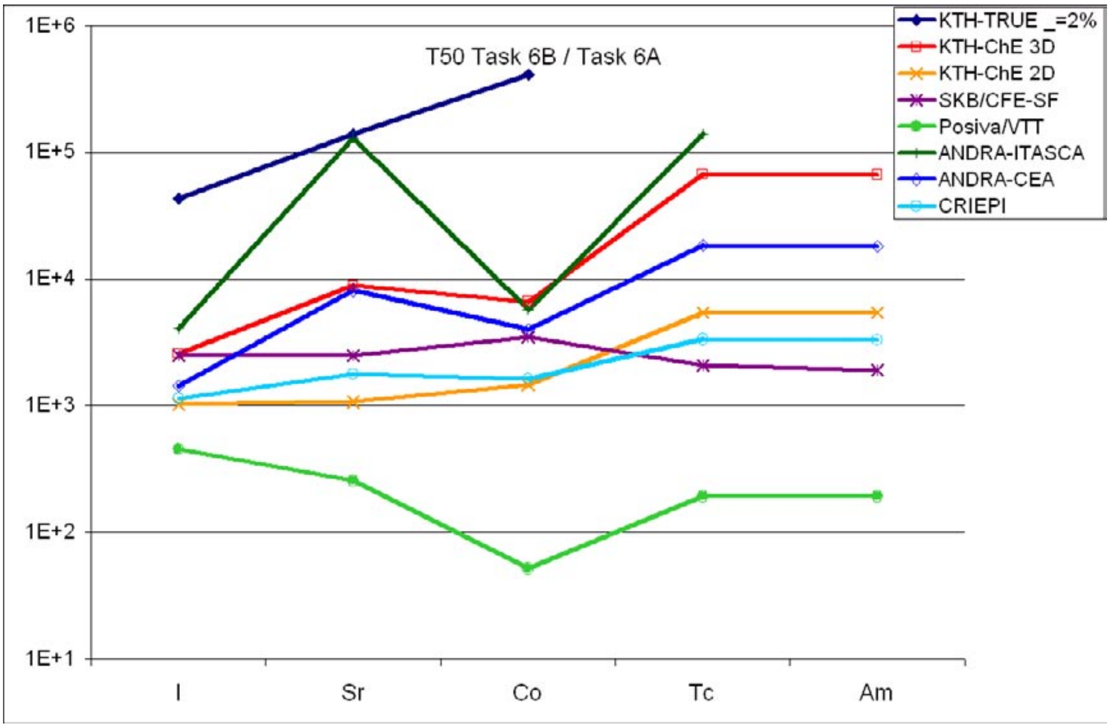

Figure 4-4. Compendium of results for the 50% breakthrough time (y) for a Dirac pulse for Task 6B results divided by Task 6A results.

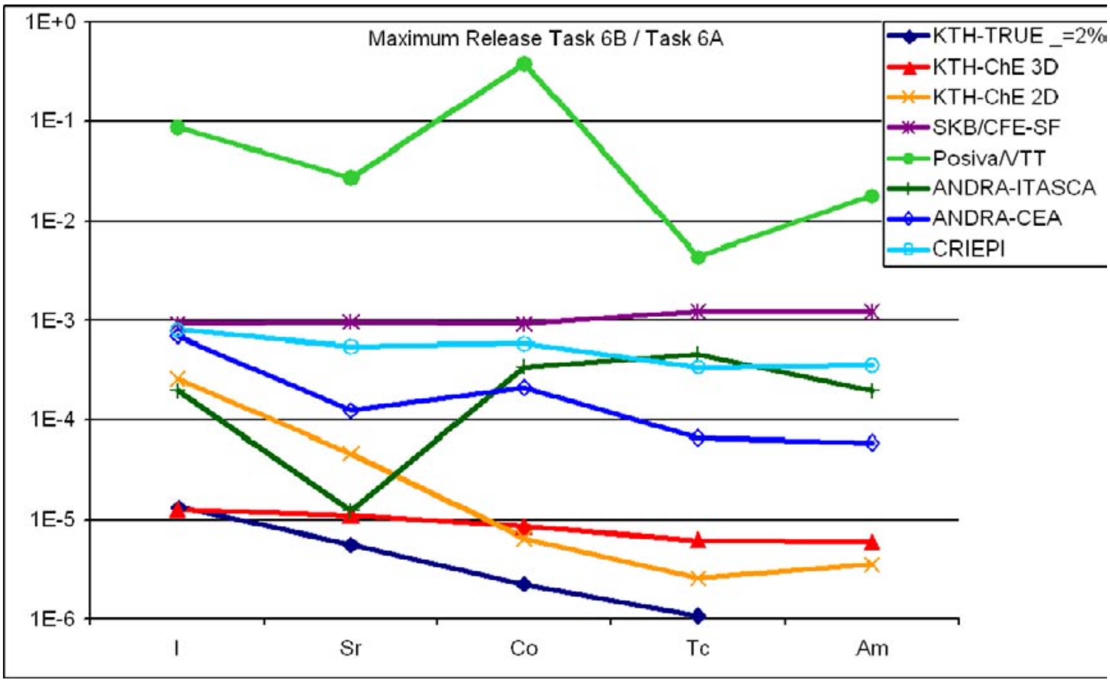

Figure 4-5. *Compendium of results for the maximum release rate (1/y) for a Dirac pulse for Task 6B results divided by Task 6A results.*

With the same approximations, it can be shown from the analysis in /Poteri, 2004/ that the maximum release rates for 6B relative to 6A are approximately given by:

$$\text{Max B} / \text{Max A} \approx t50\,[A] / t50\,[B], \qquad (4.4)$$

which implies that Figure 4-5 is the inverse of Figure 4-4 for the strongly sorbed elements. Inspection of Figures 4-4 and 4-5 shows that (4.4) is a reasonable guide for a number of models.

While only approximate, equations (4.3) and (4.4) provide general guidance for understanding the spread of results for strongly sorbing elements in Figures 4-4 and 4-5, and thereby the extrapolation of SC results to PA timescales.

It would be possible to derive improved formulae by considering an analytical model with two finite-thickness layers with different transport properties. This could then be used to summarise the results of the various analyses and to provide a sound basis for understanding the extrapolation of transport results from SC to PA timescales.

4.2.3 Task 6B2

Figure 4-6 and 4-7 show the ratio of some deterministic Task 6B2 results to Task 6B results for t50 and the maximum release rate. These figures illustrate the effect of changing the boundary conditions from convergent radial flow to a borehole to linear flow between a line source and a line sink. Also, for some of the groups, changes in modelling assumptions have been made between the two cases.

By and large, where the major change between 6B and 6B2 is just the altered geometry, the 6B2 results are within about an order of magnitude of 6B are within about an order of magnitude. Where there are larger differences between 6B and 6B2, these are due to changes in modelling assumptions. For example, the ANDRA-CEA results show large differences between 6B and 6B2. These results compare the central case of their PA model for Task 6B2 with the results of their SC model for Task 6B, which has different characteristics. Thus Figures 4-6 and 4-7 do not provide a meaningful comparison of the ANDRA-CEA results. Extensive sensitivity analyses have been carried out by /Grenier, 2004/, which allows a detailed understanding of the ANDRA-CEA results.

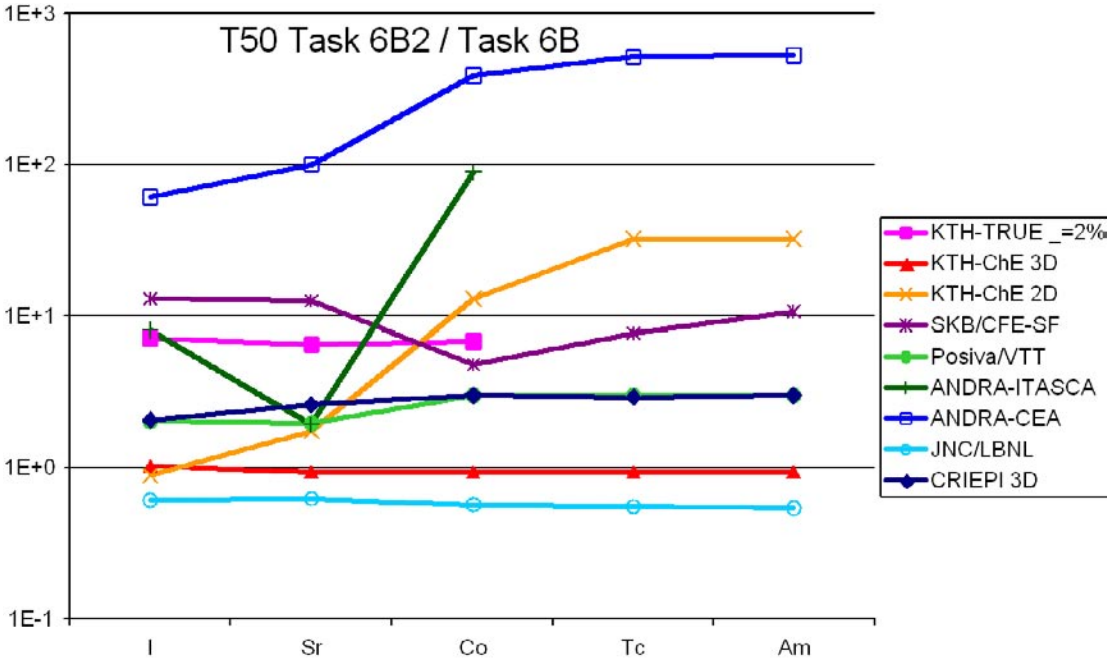

Figure 4-6. *Compendium of results for the 50% breakthrough time (y) for a Dirac pulse for Task 6B2 results divided by Task 6B results.*

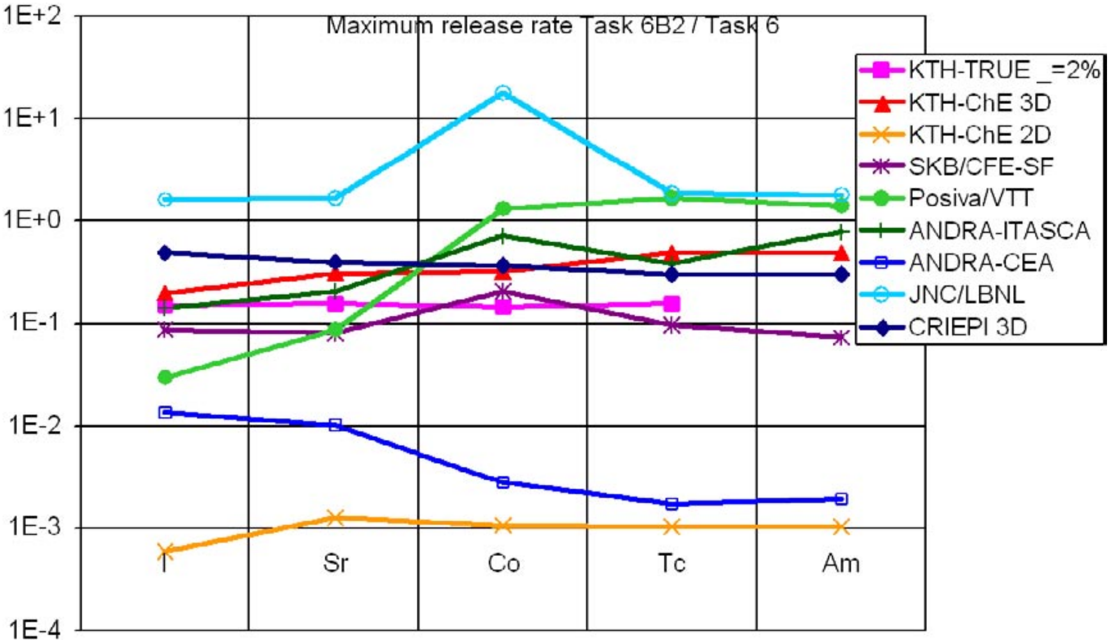

Figure 4-7. *Compendium of results for the maximum release rate (1/y) for a Dirac pulse for Task 6B2 results divided by Task 6B results.*

As discussed in Section 3.3, the probabilistic approach of the ANDRA-Golder team /Holmén and Forsman, 2004/ provides a useful way of quantifying the constraining power of tracer tests. Figures 4-8 and 4-9 provide examples of their results. These figures show cumulative probability distributions of the arrival time and size of the largest peak in mass flow, for a Dirac pulse injection of strontium. The difference between the curves for the given and constrained coupled parameter distributions shows the quantitative constraining power of the tracer tests on PA results. Essentially the conditioning leads to realisations in which on average the timescale of Sr breakthrough is reduced, the peak mass flow is increased and the range of predicted values is reduced compared with realisations that did not take into account the information from the tracer experiments. Thus the information from the tracer experiments has allowed the definition of a region of parameter space that is consistent with both the experimental data and the other data sources used to construct the given parameter distributions.

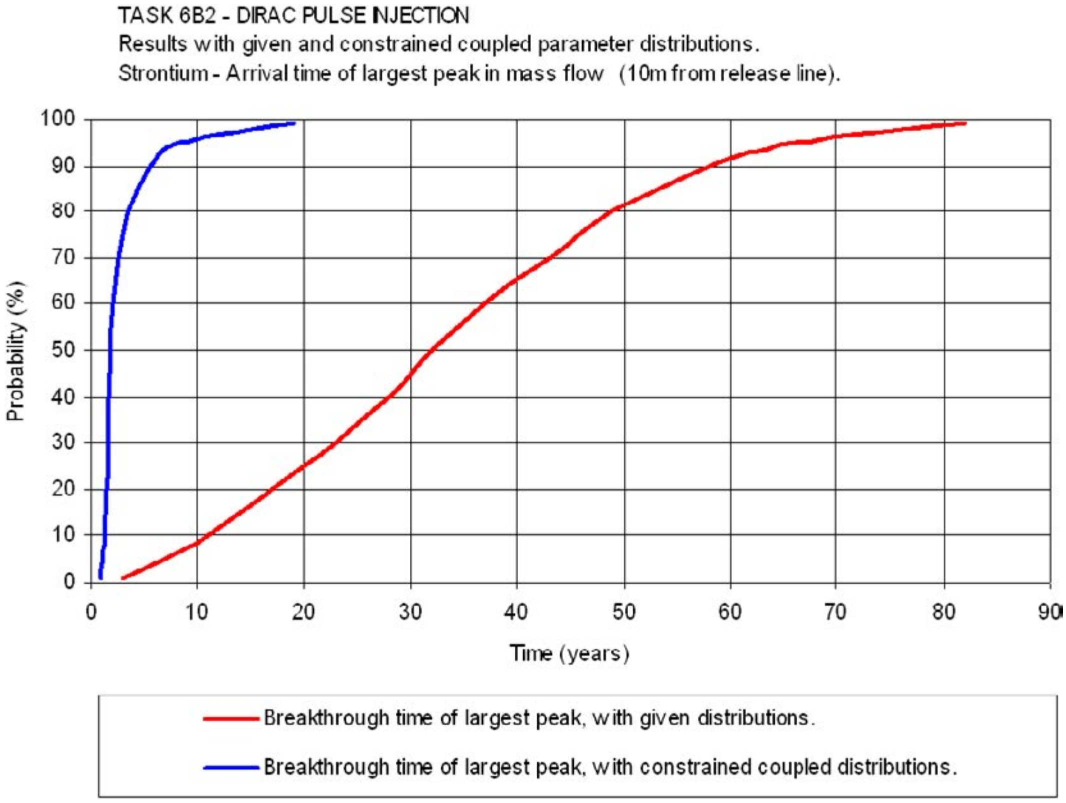

Figure 4-8. *Probability distributions of arrival time for the largest peak in mass flow for strontium in Task 6B2 with a Dirac pulse injection /Holmén and Forsman, 2004/.*

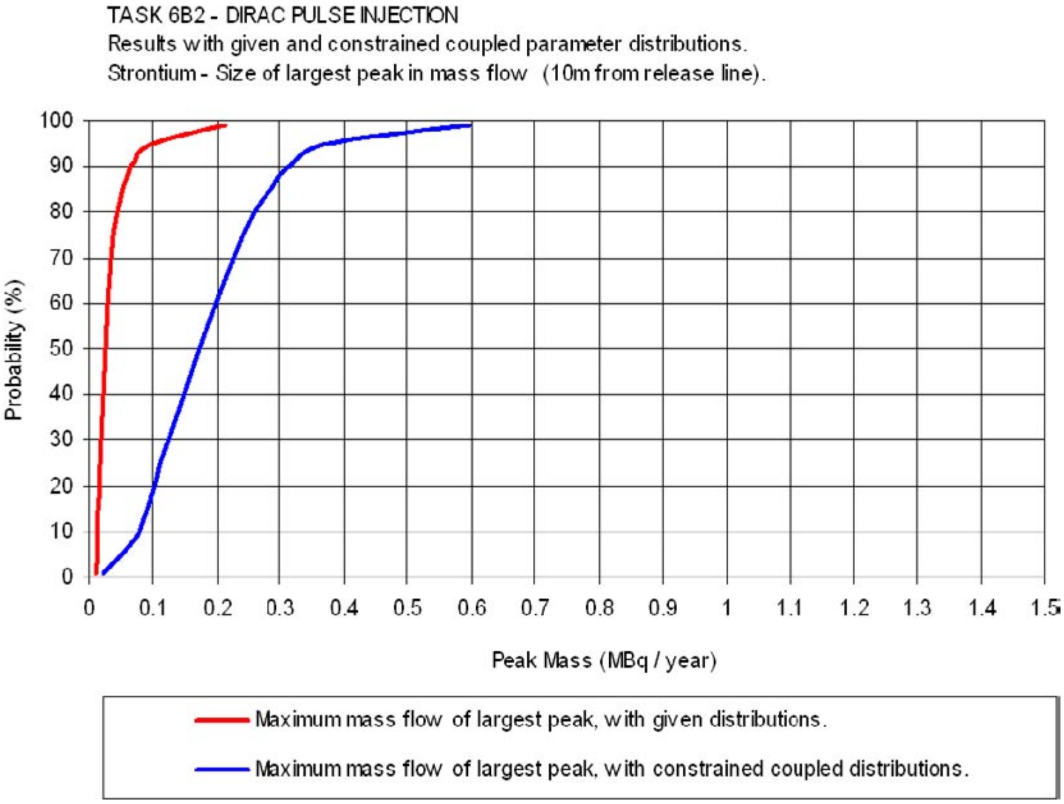

Figure 4-9. *Probability distributions of size of the largest peak in mass flow for strontium in Task 6B2 with a Dirac pulse injection /Holmén and Forsman, 2004/.*

5 Conclusions and recommendations

Task 6 is based on extensive and well documented hydraulic and tracer data supported by extensive laboratory data. It addresses the important and challenging issue of how to bridge the gap between SC and PA modelling of tracer transport in fractured rocks. The Äspö Task Force provides an excellent forum for addressing these challenges by bringing together the integrated expertise of experienced experimentalists and mathematical modellers within an international collaborative project. This section addresses the questions.

- What have we learnt (Section 5.1)?
- What are the implications for the Task 6 objectives (Section 5.2)?
- Where do we go from here (Section 5.3)?

Section 5.1 has benefited from discussions at Task Force meetings, in particular the interactive session at the 19th Task Force meeting at Naantali in Finland.

5.1 What have we learnt?

5.1.1 Flow

The quantitative description of water flow within and around Feature A still needs further refinement from the perspective of building confidence in a repository safety case, although it is likely to be adequate for performance assessment studies.

This is reflected in the fact that most teams modelled Feature A as a single planar fracture despite some qualitative evidence to the contrary. Some teams accounted for channelling within the fracture plane due to transmissivity variability, but there is currently insufficient data to properly support such models.

Only one team (JNC-LBNL) attempted to model the small-scale three-dimensional hydraulic sub-structure of Feature A explicitly. This approach could provide a useful testing ground for understanding flow in complex fractures. For example, it is possible that where features consist of pseudo-parallel fractures, flow tends to jump between them and so is generally only in one fracture at a time.

For the other approaches the gap in understanding of the flow field on a mm and cm scale was essentially bridged by modelling assumptions. For example, a phenomenological flow aperture and a phenomenological transport aperture are often defined, but their precise relationship remains an open issue. Also, the flow-wetted surface (FWS) concept is often used but it depends on the flow path of the specific system and so is not rigorously defined. FWS is essentially an engineering approach, for example of relevance to heat exchangers where the geometry is reasonably well specified. The complexity and unbounded nature of geological features makes it very difficult to relate FWS to fundamental properties of the rock mass. Small-scale flow-related information will eventually be needed to demonstrate understanding of the system, for example the proposed resin injection experiments and detailed flow logging are likely to throw light on these issues.

Also, only one team (SKB-KTH-ChE) modelled the three-dimensional flow connectivity with the surrounding rock mass. While the relatively high transmissivity and the large experimental pressure gradient ensured that most of the flow in the tracer test was along the one or two fault planes in Feature A, this will not necessarily be the case under natural long-term conditions.

In principle, tracer dilution data could be used as a further constraint on modelling the flow system. However, in practice this involves essentially arbitrary decisions about contributions from other pathways.

With the current state of knowledge, it is important to keep an open mind about the conceptualisation of flow in low permeability sparsely fractured rock. There are indications that flow may take place in relatively few discrete channels, rather than flow spread over the planes of fractures that are reasonably well connected.

An impressive range of conceptual and mathematical flow models was used in the study. In general all teams were able to calibrate their different models to the water travel time and dispersion for non-sorbing tracers. This demonstrates that the hydraulic data is not yet sufficient to discriminate between models.

However, it can be argued that Tasks 6A, 6B and 6B2 were primarily focussed on pore space interactions, with the flow field essentially specified, and thus it was not appropriate to direct too much effort towards the flow field.

5.1.2 Pore space interactions

A major achievement of the work reviewed here is the development of a consensus about the general conceptual model for diffusion and sorption of tracers into a range of pore spaces with different transport characteristics.

The modelling teams used a number of implementations of this conceptual model, and various methodologies were used to condition the models to the laboratory and field data. For example, Task 6 participants considered models with different immobile zones either parallel to or perpendicular to the main fracture. Both of these modelling approaches are clearly simplifications of a complex situation where different pore spaces with complex geometries are present at different places along the feature. There is clearly scope for developing further representations that capture the essence of the process interactions and are not unnecessarily complex. Nevertheless there was general agreement that short-term tracer tests only constrain the parameters of the most accessible pore spaces. Conversely, the rock matrix properties required for long-term performance assessments are not significantly constrained by such tests and need to be measured independently.

There is considerable documented geological evidence for the occurrence of pore space diffusion in the TRUE-1 block and at other locations, which provides a sound basis for the inclusion of this process by the modelling teams. Also, many analyses have deduced the action of matrix diffusion based on inverse power law tailing of tracer breakthrough curves. However, large effective values of diffusivity derived from such tailing can under some circumstances be due to hydrodynamic dispersion due to tracer advection between slow and fast channels. Thus it would have been useful to have documented the reasons for assuming that the primary mechanism under the conditions of Tasks 6A, 6B and 6B2 is diffusion rather than dispersion.

Knowledge of the value of the β parameter is a major uncertainty in the modelling of tracer tests and in regard to extrapolating tracer migration to PA time scales. In particular it appears that this uncertainty is a major contributor to the wide range of results with increasing sorption calculated by the different modelling teams. Moreover, there is currently little understanding of how the β parameter might vary between experimental and PA time scales.

With hindsight it would have been useful if more quantitative information about the immobile zones had been available. This would have narrowed the range of implementations of the basic conceptual model.

All of the groups assumed that sorption can be adequately modelled by a K_d factor representing linear equilibrium reversible process. This may be a reasonable assumption for PA calculations, although if the PA aims to be realistic then permanent fixing of species into mineral structures may need to be considered. However, on experimental timescales kinetic effects may be important. Also, it can be argued that the K_d approach is a way of describing sorption rather than explaining it. Thus it is appropriate to continue to pursue research into more fundamental approaches to modelling retention processes.

5.1.3 Tracer testing

As tracer tests only measure short-term behaviour, in future site characterization studies they should perhaps be used primarily with conservative tracers to establish connectivity, water travel time and dispersivity, rather than to study radionuclide transport processes.

However, sorbing tracer tests have proved useful in demonstrating that it is not appropriate to use laboratory K_d values to interpret field tracer experiments, and that using laboratory values does not over-estimate sorption. Also, they have been important in understanding behaviour in and near fractures. Thus there is a case for continuing to carry out some tracer tests with sorbing tracers.

The radially converging test configuration has proved valuable because there is a good possibility that all of the tracer is recovered, thereby reducing the ambiguity of the interpretation. It would be helpful in reducing the degrees of freedom of the interpretation if experiments could be carried out with more than one flow rate. However, in practice it has proved difficult to carry out experiments with significantly different flow rates.

A key problem with tracer tests is the need to overcome the background flow. Thus it would be best to perform them where background flows are small, for example away from the immediate vicinity of drifts or using boreholes drilled from the surface.

It would be useful to carry out tracer tests in less transmissive fractures that are more representative of the averagely fractured rock. Some tests of this type are currently being performed as part of the TRUE Block Scale continuation programme.

5.1.4 Inverse modelling methodology

The probabilistic approach of the ANDRA-Golder team was successful in investigating a large section of parameter space and in propagating parameter correlations to performance assessment. It would have been interesting to have performed a cluster analysis of the selected solutions to see if they fell into reasonably well-defined conceptual model classes.

As demonstrated by the JNC-Golder team, it is useful to constrain theoretically-motivated parameter groups rather than individual parameters.

5.1.5 Forward transport modelling

While most groups assumed a single fracture geometry, with or without stochastic variability, based on the quantitative data in the specification, the JNC-LBNL group successfully incorporated the qualitative geological structure information on the complexity of features from /Mazurek and Jacob, 2002/, thereby enhancing the realism of the conceptual model. However, for PA modelling a valid approach is to use a simple fracture geometry and to represent the detailed processes using effective parameters. Information on the complexity of features and the derivation of the effective parameters is then included in the supporting description of the state of knowledge.

Task 6 is providing important arguments for safety cases, primarily in the area of retention in immobile zones.

5.1.6 Forming a bridge between SC and PA modelling

Tasks 6A, 6B and 6B2 have been a useful learning exercise relating to the process of forming a bridge between SC and PA modelling. They illustrate that while laboratory and field characterisation data and associated SC modelling is necessary, it is rarely sufficient for PA. The key reason for this is that site characterisation can only quantify relatively short-term phenomena. Information or assumptions about long-term processes, for example from natural analogues, is also required.

The bridge building process is very important. We need to prove understanding, demonstrate that it is viable, check its consistency and subject it to independent review.

One problem with relatively complex SC models is that it is difficult to present the arguments clearly. Thus there will always be a need for simple bounding calculations.

In addition to the use of simplified PA models, there is a need to improve understanding of some processes and concepts in order to improve the level of confidence within the scientific community. In particular, the relationship of the β parameter, transport aperture and K_d to more fundamental considerations requires further study.

5.1.7 International modelling projects

The international collaboration dimension of the Task Force has been a key element in its success. It has provided a useful forum for the exchange of ideas among a peer group from similar organisations in different countries. For example this has led to an improved understanding of immobile zone interactions and has raised and discussed unresolved issues such as the β parameter. The Task Force also provides a useful training ground for researchers new to the field.

Over the past 15–20 years there have been significant advances in this field, and the Task Force has contributed significantly to these. However, care needs to be taken to ensure that the Task Force does not form a consensus that is blind to other perspectives. The commissioning of independent reviews, such as the present report, helps to guard against this possibility.

There is a need to communicate the work of the Task Force to the scientific community, and thus it would be beneficial if there were more presentations of Task Force work at conferences, and papers published in peer-reviewed journals.

The manner in which the Task Force is conducted is an important ingredient of its success. The Task Force is a very civilised forum where due respect is given to alternative views. Sometimes this can manifest itself as a lack of discussion and argument following presentations. However, the meetings clearly have an impact on the work of the modelling groups, for example in modifications to approaches presented at subsequent meetings.

The exercise reviewed here can be viewed as a form of integrated conceptual model sensitivity study of the residual uncertainty remaining after the system has been constrained by tracer test data and other site characterisation information. One disadvantage of such an exercise being carried out as part of an international project is that the modelling teams act rather independently of each other. For the future it might be worthwhile to consider stronger coordination, for example a task leader or core group who could steer the exercise on a more frequent basis than was possible at the Task Force meetings.

5.2 What are the implications for the Task 6 objectives?

On the scale of Feature A, the implications for the Task 6 objectives are as follows.

1. Assessment of simplifications used in PA models

a. Identification of the key assumptions and the less important assumptions for long-term PA predictions

Key assumptions for long-term PA predictions are the general characteristics of the water flow paths and the extent to which dissolved radionuclides can diffuse and sorb within the rock matrix.

If it is assumed that flow from a repository only occurs along a network of paths similar to the fault plane(s) within Feature A then this could considerably underestimate the degree of interaction of radionuclides with the rock mass. This may be reasonable if a pessimistic philosophy is adopted in the PA, but increasingly PAs and associated safety cases are tending to adopt more realistic approaches. If a more realistic approach is to be adopted then account needs to be taken of the hydraulic sub-structure of features such as Feature A, and connectivity with fractures in the surrounding rock mass.

As demonstrated by the results of the modelling teams, a key assumption is to distinguish between the diffusion parameters derived from short-term tracer tests and those required for PA.

b. Identification of the most significant PA model components of a site

The most significant PA model components of the site identified in this exercise are the characteristics of the flow paths, and the diffusive and sorptive properties of the intact rock matrix. By comparison, the diffusive and sorptive properties of near-fracture immobile zones, which dominate the interpretation of short term tracer tests, are not important for PA.

c. Prioritisation of PA modelling assumptions and demonstration of a rationale for simplification of PA models by parallel application of several PA models of varying degrees of simplification

The highest priority modelling assumption concerns the general geometry and connectivity of flow paths within the rock mass. However, this was not the primary focus of the current exercise.

Within Tasks 6A, 6B and 6B2 the modelling teams have demonstrated that the key modelling assumptions concern the conceptualisation and representation of the range of pore space properties as a function of distance into the rock. Moreover, a number of teams have demonstrated that a suitable PA representation is to incorporate all the rapid near-fracture processes into an effective surface retardation coefficient, and the slower processes via a one-dimensional diffusion/sorption equation into the intact rock.

d. Provision of a benchmark for comparison of PA and SC models in terms of PA measures for radionuclide transport at PA temporal and spatial scales

Tasks 6A, 6B and 6B2 provide a suitable benchmark and PA measures on a scale of about 5 metres. The modelling specifications are well formulated and relevant numerical performance measures were specified, but it would also have been useful to specify some non-numerical performance measures including the topics to be included in the modelling team reports, such as the implications for the Task 6 objectives. A positive feature of this exercise is that modelling teams have applied a wide range of different conceptual and mathematical models of varying complexity. This diversity contributes to a greater depth of understanding of transport in fractured rock.

e. Establishment of a methodology for transforming SC models using site characterisation data into PA models in a consistent manner

The methodologies used by the modelling teams included deterministic best fits of model parameters to test data, with and without sensitivity analysis, and probabilistic sensitivity analysis. Some form of sensitivity analysis is appropriate for providing input to PA in order to propagate appropriate uncertainties.

However, if parameters are represented by uncorrelated distributions, when in reality they should be correlated, then this would give rise to implausible combinations of parameters and the overall PA uncertainty would be over-estimated. A practical solution to this problem has been advocated by the ANDRA-Golder team in terms of a probabilistic sensitivity analysis methodology that propagates vectors of parameter combinations, which are consistent with experiments, to PA.

A further way to deal with the issue of correlations is to carry out the analysis in terms of theoretically-motivated parameter groups rather than for the individual model parameters. For example, the JNC-Golder team found that for Task 6A the physical parameters of the solute transport model were not well constrained, but parameter groups such as the mobile/immobile volume ratio were reasonably constrained.

2. To determine how, and to what extent, experimental tracer and flow experiments can constrain the range of parameters used in PA models

Short-term tracer tests are generally performed in high transmissivity features in order to achieve results in a reasonable time. Such features, including Feature A, are not necessarily representative of the rock mass as a whole. Thus the results from such experiments do not necessarily constrain the range of fracture flow parameters required for PA, unless a pessimistic approach is adopted.

For pore space interactions it has been demonstrated by the modelling teams that short-term tracer tests only provide limited constraints on the parameters to be used for PA, because the diffusive transport parameters close to fracture surfaces in general differ from those of the intact rock accessed on longer time scales.

The most comprehensive and quantitative assessments of the degree to which the tracer tests constrain prior model parameter distributions and the subsequent PA calculations, have been made by the ANDRA-Golder and JNC-Golder teams, as illustrated in Table 4-1 and Figures 4-8 and 4-9.

3. To support the design of site characterisation programmes to assure that the results have optimal value for performance assessment calculations

Site characterisation programmes should include direct measurements of the diffusion and sorption parameters of the intact rock matrix.

The β parameter has been shown to be a critical parameter for understanding the transport of solutes in fractured rock. However, at present it is not defined in a model-independent way and is poorly characterised. New ways need to be found to derive reliable estimates for the interaction parameter between flow and diffusion under SC conditions. For example, resin injection and detailed flow-logging are likely to be able to provide useful information.

4. To improve the understanding of site-specific flow and transport behaviour at different scales using site characterisation models

Safety cases need to demonstrate confidence in the scientific basis of PA. Accordingly there is a need to develop a more quantitative understanding of flow within the sub-structure of features such as Feature A by combined experimentation and modelling. The present exercise has taken a useful step along this path, but more work is required in this area to throw greater light on the characteristics and effects of phenomena such as flow channelling, multiple near-parallel fractures, and the β parameter.

5.3 Where do we go from here?

Task 6 is successfully building a bridge between site characterization and performance assessment approaches to solute transport in fractured rock. Also there are other initiatives in the wider radioactive waste community that are bringing SC and PA concepts closer together. In particular the NEA and IAEA have advocated the development of a safety case aimed at building confidence in repository safety arguments. Also, there is a discernable trend within the PA community, for example within the EC NF-PRO project, to make performance assessments more realistic. This is being achieved by integrating all available knowledge in order to build confidence that the evolution of the system is reasonably understood, and not just focussing on demonstrating reasonable compliance with radiological constraints. This trend to more realistic PA and closer integration of SC, research and PA models provides the background to the recommendations discussed below.

The foundation of all solute-transport modelling is a sound understanding of the hydraulic characteristics and geometry of the flow paths. Even for a feature of the limited size of Feature A, which has been extensively characterised, there remain many open questions as to the detailed flow characteristics and geometry. It is thus recommended that flow through and around Feature A, or a similar structure, is investigated in greater detail both experimentally and through more detailed modelling studies to throw greater light on issues such as flow channelling, flow within the thickness of the feature and the β parameter.

Feature A lies at the high end of the spectrum as regards transmissivity and connectivity at Äspö. Accordingly it is recommended that in addition similar studies are made of features in the middle of the spectrum, in the so-called averagely fractured rock.

The connectivity of the rock mass as a whole is also of relevance. For example, there are indications of compartmentalisation of flows at Äspö and at other low permeability crystalline rock sites, which might usefully be addressed in future by the Äspö Task Force.

The present exercise has significantly improved the state of knowledge of how flowing tracers interact with stagnant pore spaces. However, the analysis of diffusion and sorption into these pore spaces is complicated by the fact that the water is moving rapidly in channels of unknown geometry and with poorly characterised β parameter. To probe the diffusive transfer and chemical interactions in the rock matrix more deeply it would be advantageous to separate flow from diffusive transport by analysing experiments in which stationary tracer solutions are kept in contact with fracture surfaces of known area. Moreover, such experiments could also be used to make a more in-depth analysis of the chemical interactions between solutes and rock, making use of reactive geochemical transport codes. In order to address long-term issues it would also be useful to apply such models to the analysis of natural analogue data for near-fracture chemical alteration.

Acknowledgement

We would like to thank the Task Force secretariat for their help and support in conducting this review, and the Task Force participants for their openness and forbearance during the review process.

References

Abelin H, Neretnieks I, Tunbrant S, Moreno L, 1985. Final report of the migration in a single fissure – Experimental results and evaluation, Stripa Project Technical Report 85-03. Svensk Kärnbränslehantering AB.

Abelin H, Birgersson L, Widén H, Ågren T, Moreno L, Neretnieks I, 1990. Channeling experiment. Stripa Project Technical Report TR 90-13. Svensk Kärnbränslehantering AB.

Altman S J, Uchida M, Tidwell V C, 2000. Visualization and quantification of heterogeneous diffusion rates in granodiorite samples by X-ray absorption imaging: Diffusion within gouge materials, altered rim and intact rock. Sandia National Laboratories, SAND2001-0743C.

Andersson P, Wass E, Johansson H, Skarnemark G, Skålberg M, 1999. Äspö Hard Rock Laboratory, TRUE 1st Tracer test programme, tracer tests with sorbing tracers, STT-1b, Experimental description and preliminary evaluation. SKB IPR-99-12. Svensk Kärnbränslehantering AB.

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

Andersson P, Byegård J, Winberg A, 2002b. Final Report of the TRUE Block Scale Project: 2. Tracer tests in the block scale. SKB Technical Report TR-02-14. Svensk Kärnbränslehantering AB.

Bäckblom G, Olsson O, 1994. Program for Tracer Retention Understanding Experiments. PR 25-94-24. Svensk Kärnbränslehantering AB.

Becker M W, Shapiro A M, 2000. Tracer transport in fractured crystalline rock: Evidence of nondiffusive breakthrough tailing. Water Resources Research, Vol. 36, No. 7, pp 1,677–1,686.

Becker M W, Shapiro A M, 2003. Interpreting tracer breakthrough tailing from different forced-gradient tracer experiment configurations in fractured bedrock. Water Resources Research, Vol., 39, No. 1, pp 1,024–1,036.

Benabderrahmane H, Dershowitz W, Selroos J-O, Uchida M, Winberg A, 2000. Task 6: Performance Assessment Modelling Using Site Characterisation Data (PASC), November 28, 2000.

Billaux D, Paris B, 2001. 3FLO Version 2.0 – Calculs d'écoulements et de transport tridemensionnels. Volume 3 – Bases théoriques. Internal report ITASCA Consultants.

Billaux D, 2004. Äspö Modelling Task Force: Task 6A and 6B Modelling. International Progress Report IPR-04-40 (Draft). Svensk Kärnbränslehantering AB.

Black J H, Robinson P C, Barker J A, 2005. A Preliminary Investigation of the Concept of Hyper-convergence using Sparse Channel Networks. In Situ Solutions report ISS 2003-3 for SKB.

Bourke P J, 1987. Channelling of flow through fractures in rock, Ed: A Larsson, Proceedings of the SKI/NEA GEOVAL-1987 Symposium, 167–177.

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

Byegård J, Widestrand H, Skålberg M, Tullborg E-L, Siitari-Kauppi M, 2001. Complementary investigations of diffusivity, porosity and sorptivity of Feature A – site specific material. ICR-01-04. Svensk Kärnbränslehantering AB.

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

Cheng H, Cvetkovic V, 2004. Äspö Task Force. Tasks 6A, 6B and 6B2: Modelling of Sorbing Tracer Breakthrough for Tasks 6A, 6B and 6B2. International Progress Report IPR-04-30 (In press). Svensk Kärnbränslehantering AB.

Crawford J, Moreno L, 2004. Task 6A and 6B/6B2. Modelling of the STT-1b Detailed Scale Tracer Tests at Äspö using the Channel Network Model: International Progress Report IPR-04-31 (In press). Svensk Kärnbränslehantering AB.

Crawford J, 2004. Private communication.

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

Cvetkovic V, Cheng H, Selroos J-O, 2000. Evaluation of Tracer Retention Understanding Experiments (first stage) at Äspö. International Cooperation Report, ICR-00-01, SKB.

Dershowitz W, Winberg A, Hermansson J, Byegård J, Tullborg E-L, Andersson P, Mazurek M, 2003. Äspö Hard Rock Laboratory, Äspö Task Force on modelling of groundwater flow and transport of solutes, Task 6C, A semi-synthetic model of block scale conductive structures at the Äspö HRL. International Progress Report IPR-03-13. Svensk Kärnbränslehantering AB.

Dershowitz W, Shuttle D, Uchida M, 2004. Task 6A, 6B and 6B2. GoldSim and FracMan/LTG Modeling: Performance Assessment Modeling Using Site Characterisation Data (PASC). International Progress Report IPR-04-32 (In press). Svensk Kärnbränslehantering AB.

Doughty C, Uchida M, 2004. PA Calculations for Feature A with Third-dimension Structure Based on Tracer Test Calibration. International Progress Report IPR-04-33 (In press). Svensk Kärnbränslehantering AB.

Elert M, 2003. Summary of Tasks 6A, 6B & 6B2. Presentation at Äspö Task Force Workshop, Krägga, Sweden, September 2003.

Elert M, Selroos J-O, 2001. Task 6B2 Modelling Task Specification. Version 1.0. Äspö Task Force Technical Note, 7 December 2001.

Elert M, Selroos J-O, 2004. Task 6D specification of additional performance measures. Version 1.0, Äspö Task Force Technical Note, 6 February 2004.

Elert M, Svensson H, 1999. Äspö Hard Rock Laboratory: Deconvolution of breakthrough curves from TRUE-1 tracer tests (STT-1 and STT-1b) with sorbing racers: Äspö Task Force, Task 4E. International Progress Report IPR 99-35. Svensk Kärnbränslehantering AB.

Elert M, Svensson H, 2001. Evaluation of modelling of the TRUE-1 radially converging tests with sorbing tracers: The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes: Tasks 4E and 4F. SKB TR-01-12, Svensk Kärnbränslehantering AB.

Grenier C, 2004. Modelling Transfers in a Single Fracture System: From Site Characterisation to Performance Assessment Models. Contribution to Task 6A and 6B from the Äspö Modelling Task Force Exercise. International Progress Report IPR-04-37 (Draft). Svensk Kärnbränslehantering AB.

Gustafson G, Ström A, 1995. The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes: Evaluation Report on Task No 1, the LPT2 large scale field experiments. International Cooperation Report ICR 95-05. Svensk Kärnbränslehantering AB.

Gustafson G, Ström A, Vira J, 1997. The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes: Evaluation Report on Task No 3 – The Äspö Tunnel Drawdown Experiment. International Cooperation Report ICR 97-06. Svensk Kärnbränslehantering AB.

Gylling B, 1997. Development and Applications of the Channel Network Model for Simulation of Flow and Solute Transport in Fractured Rock. Ph.D. Thesis, Department of Chemical Engineering and Technology, Royal Institute of Technology.

Gylling B, Birgersson L, Moreno L, Neretnieks I, 1998. Analysis of a long term pumping and tracer test using the Channel Network Model. Journal of Contaminant Hydrology, 32: pp 203–222.

Hakami E, 1995. Aperture distribution of rock fractures. PhD-thesis TRITA-AMIPHD1003. Royal Institute of Technology (KTH), Stockholm, Sweden.

Hakami E, Larsson E, 1996. Aperture measurements and flow experiments on a single natural fracture. Int. J. of Rock Mech. and Mining Sciences & Geomech. Abstr., vol. 33, no 4, pp 395–404.

Hakami E, Gale J, 1999. First TRUE Stage – Pilot Resin Experiment – Pore space analysis. Äspö HRL International Progress Report IPR-99-14. Svensk Kärnbränslehantering AB.

Hodgkinson D P, Lever D A, 1983. Radioactive Waste Management and the Nuclear Fuel Cycle, Volume 4(2), pp 129–158.

Holmén J, Forsman J, 2004. Äspö Modelling Task Force: Modelling of Task 6A and Task 6B2. International Progress Report IPR-04-39 (Draft). Svensk Kärnbränslehantering AB.

Jacob A, 2004. Matrix Diffusion for Performance Assessment – Experimental Evidence, Modelling Assumptions and Open Issues. Paul Scherrer Institut report 04-08, ISSN 1019-0643.

Jakob A, Heer W, 2000. Summary of work done by the PSI modelling team for the Äspö migration experiments, Tasks 4E and 4F. Paul Scherrer Institute Technical Note TM-44-00-01.

Kawanishi M, Igarashi T, Mahara Y, Komada H, Maki Y, 1987. Computer models for safety assessment on land disposal of low-level wastes. Waste Management '87, 3, pp 175–180. Tucson, Arizona.

Marschall P, Elert M, 2003. Overall evaluation of the modelling of the TRUE-1 tracer tests – Task 4: The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes. SKB TR-03-12, Svensk Kärnbränslehantering AB.

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

Mazurek M, Jacob A, 2002. Evidence for matrix diffusion in the TRUE-1 Block at Äspö based on fracture characterization and modeling of tracer tests, in: Radionuclide Retention in Geologic Media, Workshop Proceedings, Oskarshamn, Sweden, 7–9 May 2001, Nuclear Energy Agency, Paris, France, OECD 2002, 137–154.

Moench A, 1989. Convergent radial dispersion: a Laplace transform solution for aquifer tracer testing. Water Resources Research, Vol. 25, No. 3, pp 439–447.

Moreno L, Tsang Y W, Tsang C F, Hale F V, Neretnieks I, 1988. Flow and tracer transport in a single fracture: A stochastic model and its relation to some field observations. Water Resources Research, 24: pp 2,033–3,048.

Moreno L, Neretnieks I, 1993. Fluid flow and solute transport in a network of channels, Journal of Contaminant Hydrology, 14, 163–192.

Miller I, 2002. GoldSim Pro, Version 751.1. User Documentation. Golder Associates Inc., Redmond, Washington, USA.

NEA, SKB, 1994. In Situ Experiments at the Stripa Mine: Proceedings of the Fourth International NEA/SKB Symposium, Stockholm, Sweden, October 1992.

NEA, 1999. Confidence in the Long-term Safety of Deep Geological Repositories: Its Development and Communication. OECD-NEA, Paris.

Neretnieks I, Moreno L, 2000. Analysis of the TRUE experiment considering a 3D flow-pattern. Presentation at the 14th Äspö Task Force meeting.

Neretnieks I, Moreno L, in press. Prediction of some in-situ tracer tests with sorbing tracers using independent data. Journal of Contaminant Hydrology.

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

Poteri A, 2004. Modelling of the Tasks 6A, 6B and 6B2 using Posiva streamtube approach. International Progress Report IPR-04-41 (Draft). Svensk Kärnbränslehantering AB.

Poteri A, Billaux D, Dershowitz W, Gómez-Hernández J-J, Cvetkovic V, Hautojärvi A, Holton D, Medina A, Winberg A, 2002. Final report of the TRUE Block Scale project, 3: Modelling of flow and transport, SKB Technical Report TR-02-15. Svensk Kärnbränslehantering AB.

Rhén I, Smellie J, 2003. Task force on modelling of groundwater flow and transport of solutes: Task 5 Summary report. SKB TR-03-01, Svensk Kärnbränslehantering AB.

Robinson P C, 1984. Connectivity, flow and transport in network models of fractured media. Ph.D. Thesis, St. Catherine's College, Oxford University. AERE Report. TP 1072.

Selroos J-O, Winberg A, Cvetkovic V, 1994. Design constraints and process discrimination for the Detailed Scale Tracer Experiments at Äspö – Multiple Well Tracer Experiment and Matrix Diffusion Experiment. Report ICR 94-04. Svensk Kärnbränslehantering AB.

Selroos J-O, Elert M, 2001. Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes: Task 6A & 6B Modelling Task Specification, Version 1, April 2001.

SKB, 2003. Äspö Hard Rock Laboratory: Annual Report 2002. SKB TR-03-10, Svensk Kärnbränslehantering AB.

Svensson U, Kuylenstierna H-O, Ferry M, 2003. DarcyTools-Concepts, Method, Equations and Tests. Work in Progress.

Svensson U, 2004. Modelling Subgrid dispersion: Some recommendations concerning the parameters of the subgrid model FRAME. Computer-aided Fluid Engineering AB Draft Technical Note.

Svensson U, Follin S, 2004. Simulation of Tracer Transport, Considering Both Experimental and Natural Time Scales: Äspö Task Force: Task 6A, 6B and 6B2. International Progress Report IPR-04-42 (Draft). Svensk Kärnbränslehantering AB.

Tanaka Y, 2004. Äspö Task Force: Performance Assessment Modelling Using Site Characterisation Data: Application of FEGM and FERM to Task 6A, 6B and 6B2. International Progress Report IPR-04-38 (Draft). Svensk Kärnbränslehantering AB.

Tsang Y W, Tsang C-F, 2001. A particle-tracking method for advective transport in fractures with diffusion into finite matrix blocks. Water Resources Research, 37(3), 831–835, 2001.

Tsang C-F, Doughty C, 2002. An approach to modeling solute transport in a complex fracture. Lawrence Berkeley National Laboratory Report LBNL-50537, submitted to Water Resources Research.

Vieno T, Nordman H, 1999. Safety assessment of spent fuel disposal in Hästholmen, Kivetty, Olkiluoto and Romuvaara. TILA-99, Posiva 99-07, Posiva OY.

Winberg A, 1994. Tracer Retention Understanding Experiments (TRUE) – Test Plan for the First TRUE Stage. Äspö Hard Rock Laboratory Progress Report PR 25-94-35. Svensk Kärnbränslehantering AB.

Winberg A (ed), 1996. First TRUE Stage – Tracer Retention Understanding Experiments: Descriptive structural-hydraulic models on block and detailed scales on the TRUE-1 site. Äspö Hard Rock Laboratory. International Cooperation Report ICR 96-04. Svensk Kärnbränslehantering AB.

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

Winberg A, Andersson P, Poteri A, Cvetkovic V, Dershowitz W, Hermanson J, Gómez-Hernández J-J, Hautojärvi A, Billaux D, Tullborg E-L, Holton D, Meier P, Medina A, 2003. Final report of the TRUE Block Scale project, 4: Synthesis of flow, transport and retention in the block scale. SKB Technical Report TR-02-16. Svensk Kärnbränslehantering AB.

ISSN 1404-0344
CM Digitaltryck AB, Bromma, 2005