Technical Report

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Final report of the TRUE Block Scale project

4. Synthesis of flow, transport and retention in the block scale

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Foreword

This report constitutes the fourth in a series of four final reports of the TRUE Block Scale Project, the latter run within the framework of the Tracer Retention Understanding Experiments at the SKB Äspö Hard Rock Laboratory, Sweden.

The funding organisations of the project are;

ANDRA (France)

ENRESA (Spain)

JNC (Japan)

Nirex (United Kingdom)

Posiva (Finland)

SKB (Sweden)

The work done could not have been accomplished without the active participation and effort of field characterisation crews and analysis teams from the organisations and countries involved. Their contributions and the contribution of the coordinators and staff of the Äspö Hard Rock Laboratory are also acknowledged.

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Abstract

The TRUE Block Scale project was performed at the Äspö Hard Rock laboratory as an international partnership funded by ANDRA, ENRESA, JNC, Nirex, Posiva and SKB. The project, initiated mid 1996, was divided in a series of defined stages; Scoping Stage, Preliminary Characterisation Stage, Detailed Characterisation Stage, Tracer Test Stage and the Evaluation and Reporting Stage. The specific objectives were to; 1) increase understanding of tracer transport in a fracture network and improve predictive capabilities, 2) assess the importance of tracer retention mechanisms (diffusion and sorption) in a fracture network, and 3) assess the link between flow and transport data as a means for predicting transport phenomena. Characterisation in included drilling, core logging, borehole imaging, borehole radar, 3D seismic surveys, hydraulic tests (flow logging, single hole tests, cross-hole interference tests), tracer dilution tests, hydrogeochemical analyses of groundwater samples and various types of mineralogical, geochemical and petrophysical measurements on drill core samples. Drilling and characterisation of each new borehole was followed by analysis and decision with regards to need and geometry of a subsequent borehole. The main set of tools for determining the conductive geometry and the hydrostructural model was a combination of borehole television (BIPS), high resolution flow logging and pressure responses from drilling and cross-hole interference tests. The constructed hydrostructural model was made up of a set of deterministic subvertical structures mainly oriented northwest. Hydraulic features not part of the deterministic set were included in a stochastic background fracture population. Material properties and boundary conditions were also assigned to the developed model. Characteristics and properties measured in the laboratory were integrated in generalised microstructural models. Hypotheses formulated in relation to defined basic questions were addressed in the *in situ* radioactive sorbing tracer tests and in the subsequent evaluation using numerical models. The *in situ* tracer test programme was crowned by four injections of cocktails of radioactive sorbing tracers in three different source-sink pairs over distances ranging between 15 and 100 m, as integrated along the deterministic structures of the hydrostructural model, defining flow paths of variable complexity. Numerical modelling using a variety of concepts/codes constituted an important and integrated component of the project. A major accomplishment in this context was the development of a common conceptual basis for transport and retention. The fractured crystalline rock volume was here conceptualised as a dual porosity medium (mobile-immobile). Model predictions of the sorbing tracer tests were followed by evaluation modelling where the various modelling results were used for elevating understanding of block scale transport and retention and relative role of processes. Diffusion to the immobile pore space, sorption in the immobile pore space and surface sorption on the fracture surfaces along the transport paths were interpreted as the main retention processes in the prediction and evaluation models applied. This interpretation was supported both by the characteristics of *in situ* breakthrough curves and modelling, where in the latter case the measured residence time distributions were reproduced more accurately with diffusional mass transfer invoked. Geological information from the site also provides support for the assumption of multiple immobile zones along the investigated flow paths.

Sammanfattning

Projektet TRUE Block Scale genomfördes vid Äspölaboratoriet som ett internationellt samarbetsprojekt finansierat av ANDRA, ENRESA, JNC, Nirex, Posiva och SKB. Projektet, som inleddes i mitten av 1996, delades in i ett antal definierade faser; Scoping Stage, Preliminary Characterisation Stage, Detailed Characterisation Stage, Tracer Test Stage och Evaluation and Reporting Stage. Projektets syften var att: 1) öka förståelsen av transport av lösta ämnen i nätverk av sprickor och öka förmågan att göra modellförutsägelser, 2) undersöka betydelsen av retentionsprocesser (diffusion och sorption) i spricknätverk, samt 3) undersöka kopplingen mellan flöde och transport för att bättre kunna förutsäga transportfenomen. Karakteriseringsarbetet omfattade kärnborrning (triple tube), kärnkartering, borrhåls-TV, Borrhålsradar, 3D seismik, hydrauliska tester (flödesloggning, tryckuppbyggnadstester, interferenstester), utspädningsmätningar, grundvattenanalyser och olika typer av mineralogiska, geokemiska och petrofysiska mätningar på borrkärnor. Borrning och karakterisering av varje borrhål följdes av analys och beslut avseende behov av ett påföljande borrhål och dess geometri. Huvudredskapen för att bestämma den konduktiva geometrin och den beskrivande hydrostrukturella modellen var en kombination av borrhåls-TV, högupplösande flödesloggning och tryckresponser på grund av borrning och interferenstester. Den hydrostrukturella modellen bestod av ett antal huvudsakligen nordvästliga brantstående strukturer. Övriga observerade konduktiva strukturer hänfördes till en stokastisk beskriven population av bakgrundssprickor. Vidare tillskrevs modellen materialegenskaper och randvillkor. Karakteristik och egenskaper mätta i laboratorium användes till att upprätta generaliserade mikrostrukturella modeller. Hypoteser baserade på formulerade grundläggande frågeställningar adresserades i de genomförda försöken med radioaktiva sorberande spårämnen liksom i den efterföljande utvärderingen med numeriska modeller. Försöken *in situ* kröntes med genomförandet av fyra injiceringar av sorberande spårämnen i tre olika flödesvägar, av olika komplexitet och varierade avstånd (15–100 m) längs deterministiska strukturer. Numerisk modellering med olika koncept/koder utgjorde en viktig och integrerad komponent i arbetet. En viktig prestation i detta sammanhang var framtagandet av en gemensam konceptuell plattform för transport och retention. Den studerade bergvolymen beskrevs här i termer av ett bi-poröst medium (mobil/immobil). Modellförutsägelser av försöken med sorberande spårämnen följdes av utvärdering/analys där olika resultat användes för att öka förståelsen av transport och retention i blockskala och processers relativa roll. Diffusion till immobila porvolymer, sorption i immobila porvolymer samt ytsorption på sprickytor längs flödesvägarna tolkades som de huvudsakliga retentionsprocesserna. Denna tolkning understöddes både av karakteristiska drag i genombrottskurvor och modellering, där i det senare fallet genombrottskurvor kunde reproduceras mer noggrant med diffusion inkluderad. Geologisk information från den undersökta bergvolymen stödde tolkningen av ett flertal samverkande immobila zoner längs de undersökta flödesvägarna.

Executive summary

Background and objectives

In planning the experiments to be performed during the Operating Phase of the Äspö Hard Rock Laboratory, the Swedish Nuclear Fuel and Waste Management Company (SKB) identified the need for a better understanding of radionuclide transport and retention processes in fractured crystalline rock. This understanding is a cornerstone of performance and safety assessments of the natural barrier system and it has three essential parts:

- Demonstrating the ability of numerical models to simulate transport processes involving sorbing radionuclides.

- Showing that field experiments involving practical use of site characterisation tools could identify pathways and obtain the *in situ* transport/retention data needed to characterise the flow paths through numerical simulations. This includes defining distribution coefficients, diffusion parameters and flow-related properties that govern *in situ* retention.

- Identifying approaches for integrating laboratory data on transport parameters with field-scale results at variable length scales.

To answer these needs, SKB in 1994 initiated a tracer test programme at the Äspö HRL named the Tracer Retention Understanding Experiments (TRUE) which focused on transport and retention at different length scales and at various degrees of complexity. The First Stage of TRUE was performed in the detailed scale (0–10 m) and was focused on characterisation, experimentation and modelling of an interpreted single conductive feature.

The original conceptualisation of the TRUE program recognised that transport is not confined to a single geological feature in nature. Rather, transport in natural systems involves networks of conductive features where solutes must pass through intersections, and *in situ* retention occurs in rock blocks bounded by the conductive fractures and structures. Questions persisted regarding the effects of a fracture network and its components on transport and retention. Accordingly, the original TRUE plans called for a block scale experiment involving multiple conducting features that would complement the findings of the TRUE-1 programme. The programme defined "block scale" should involve multiple conductive structures and pathway lengths in the order of about 10–100 m. Accordingly, this experimental programme was initiated as the TRUE Block Scale Project.

The specific objectives of the TRUE Block Scale Project were:

1. to increase understanding of tracer transport in a fracture network and improve predictive capabilities,
2. to assess the importance of tracer retention mechanisms (diffusion and sorption) in a fracture network,
3. to assess the link between flow and transport data as a means for predicting transport phenomena.

Rationale

The block scale is the critical region of the natural barrier system in the performance assessment approaches of many international programs. Major conducting features, such as those that produce lineaments on the ground surface or create geophysical anomalies, have spacings that are at the same scale or larger than the block scale, that is, greater than a hundred metres. Although these major conducting features may have retentive capability, some views of performance assessment attribute the major portion of the natural barrier performance to the region between waste emplacement sites and the major conductive zones. The block scale is also important from the perspective of developing repository sites.

With regards to modelling of block scale transport and retention we want to know whether our current conceptual models provide adequate descriptions of flow and transport and whether the numerical implementations of these conceptual models are adequate.

One subobjective of the block scale tracer tests is to investigate whether or not fracture intersection zones (FIZ) are regions with distinctive flow and transport properties that influence tracer migration. Although TRUE Block Scale does not provide an experimental array with the specific aim to investigate FIZs, the results from the experiments may still provide indirect evidence of the possible effects of FIZs. This hypothesis is tested by including *in situ* pathways that cross fracture or structure intersections.

Explicit evidence for the existence of gouge material (fault breccia/fine-grained fault gouge) was not found in the investigated Feature A at the TRUE-1 site. Modelling performed within the Äspö Task Force has shown that assumptions of a geologic material with increased porosity/sorption capacity in direct contact with the flowing groundwater, such as fault gouge material, can explain the observed increased *in situ* retention in TRUE-1. Fault gouge can be very fragile and difficult to recover in drill cores, even using sophisticated triple-tube coring. In the network of structures investigated as part of TRUE Block Scale, however, there is a firm evidence of fault breccia/fault gouge from the core logging.

Overview of project

The TRUE Block Scale project is an international partnership funded by ANDRA (France), ENRESA (Spain), Nirex (UK), Posiva (Finland), JNC (Japan) and SKB (Sweden) /Winberg, 1997/. The project, which was initiated mid 1996, is divided into a series of defined stages; Scoping Stage, Preliminary Characterisation Stage, Detailed Characterisation Stage, Tracer Test Stage (Phases A, B and C) and the Evaluation and Reporting Stage.

The staged approach included an iterative approach to characterisation and hydrostructural modelling, whereby the results of the characterisation of each characterisation borehole has been used to plan the subsequent borehole. The feasibility of performing tracer tests in the identified the block scale (10–100 m) network of structures was firmly demonstrated at the end of the Detailed Characterisation Stage. A series of tracer test tests followed and was crowned by the Phase C tests with radioactive sorbing tracers. The "official" monitoring in the latter case was concluded late 2000. Various laboratory investigations have been performed in support of the *in situ* experimentation. Various numerical models have been used for prediction and evaluation of the radioactive tracer tests.

Questions and hypotheses

Three basic questions were formulated at the end of the Detailed Characterisation Stage;

Q1) "What is the geometry of conductive structures of the defined target volume for tracer tests within the TRUE Block Scale rock volume? Does the most recent structural model reflect this geometry with sufficient accuracy to allow design and interpretation of the planned tracer tests?"

Q2) "What are the properties of fractures and fracture zones that control transport in fracture networks?"

Q3) "Is there a discriminating difference between breakthrough of sorbing tracers in a detailed scale single fracture, as opposed to that observed in a fracture network in the block scale?"

Hypotheses were formulated in relation to the basic questions, which were addressed in the *in situ* radioactive sorbing tracer tests and in the model predictions and subsequent evaluation.

Characterisation and hydrostructural models

Characterisation in TRUE Block Scale included drilling, core logging, borehole imaging, borehole radar, 3D seismic surveys, various types of hydraulic tests (flow logging, single hole tests, cross-hole interference tests) tracer dilution tests, hydrogeochemical analyses of groundwater samples and various types of mineralogical, geochemical and petrophysical measurements on drill core samples. Drilling and characterisation of each new borehole was followed by analysis and a decision with regards to need and geometry of a subsequent characterisation borehole. In TRUE Block Scale it was identified that an effective and reliable interpretation of conductive structures required joint evaluation of hydraulic and geologic information. The main set of tools for determining the conductive geometry and the hydrostructural model, cf Figure EX-1, was a combination of borehole television (BIPS), high resolution flow logging (Posiva difference flow log) and pressure responses (drilling/cross-hole interference tests). The hydrostructural model was made up of a set of deterministic subvertical structures mainly oriented northwest. Hydraulic conductors not part of the deterministic set were included in a background fracture population described stochastically. Material properties and boundary conditions were also assigned to the developed model.

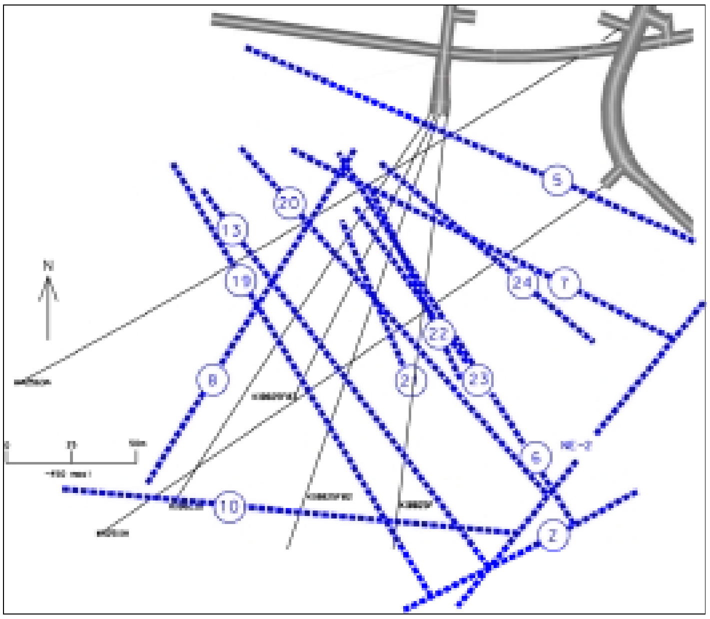


Figure EX-1. *March 2000 hydrostructural model. Plan view of interpreted deterministic structures at Z=–450 masl.*

Conceptual flow model

The hydrostructural model with associated material properties and acting hydraulic boundary conditions governs the groundwater flow in the studied rock volume. One important factor that regulates the boundary conditions is the existence of underground openings that govern the magnitude and overall direction of the hydraulic gradient. Close to the openings the hydraulic gradient is steep but in the interior of the block the gradient is flat (in the order of 0.05 m/m). The flow towards the underground openings has affected the spatial and temporal distribution of groundwater chemistry. The latter data comes from resistivity logs and analyses of groundwater samples collected from the borehole piezometers. The principal markers used to describe the origin and successive changes in ground water composition are Cl^-, ^{18}O and ^{3}H. In combination they are used to differentiate between the likely sources that are Deep brine, Baltic Seawater and Meteoric water. For example Baltic Seawater (low Cl^-, high ^{18}O and high ^{3}H) is evident in the area of Structure #10. A mix of Deep Brine and Glacial water seems to be associated with the Structure #20 and #13 system. Observations over time have mapped a progressive influx of less saline water in the area of the KA2563A intercept with Structure #20.

Characteristics of conductive fractures

Conductive structures at Äspö are associated with tectonised rock in the form of cataclasites (recrystallisation of quartz, increased frequency of micro fractures, variable degree of chemical alteration) and mylonites (complete grain size reduction, recrystallisation/alteration of wall rock). The drill cores and borehole imagery of the structures show alteration and tectonisation of the wall rock. Generally, the widths of the associated cataclastic zones are on the order of centimetres to decimetres whereas the mylonites are from millimetres to a few centimetres wide. Most structures appear to be the result of brittle reactivation of old ductile/semi-ductile deformation zones. The movements along fault planes have resulted in formation of fault breccia and fault gouge distributed in variable amounts and proportions over the fracture and structure planes. The fault gouge material is characterised in terms of grain size distribution and mineral composition. No measurements exist of *in situ* porosity of fine-grained fault gouge.

Laboratory investigations and microstructural model

Laboratory investigations included a comprehensive mineralogical and geochemical investigation of geological materials from important conductive structures. It is noted that the finest fractions (< 0.002 mm) have a high clay content and variable amounts of mixed-layer clays, illite and chlorite. The geochemical program also included analyses of stable isotopes (^{13}C, ^{18}O) and uranium series analyses on selected samples. Porosity and porosity distributions have been determined using a combination of water saturation and impregnation studies. These analyses also included cm-sized breccia pieces and mm-sized breccia fragments, apart from the wall rock of individual borehole intercepts. Impregnation studies have indicated higher porosities close to the structure walls with decreasing trends normal to the fracture surfaces. Typical porosity values and typical thicknesses of immobile zones are presented in the generalised microstructure model in Figure EX-2. K_d values of the fine-grained fault gouge were estimated using literature data on cation exchange capacities, selectivity coefficients of base minerals, site specific mineralogy and the ambient groundwater chemistry. Among the structures involved in the TRUE Block Scale tracer tests, the highest K_d for Cs (< 0.125 mm fraction) is noted for Structure #22 (0.15 m^3/kg) . This is attributed to the high clay content noted for this structure. The overall highest K_d calculated for Cs (0.28 m^3/kg) of all investigated structures is noted for Structure #19 (containing smectite). Compared to the coarser 1–2 mm fraction the K_d values are about 20–60 times higher for the finer fraction.

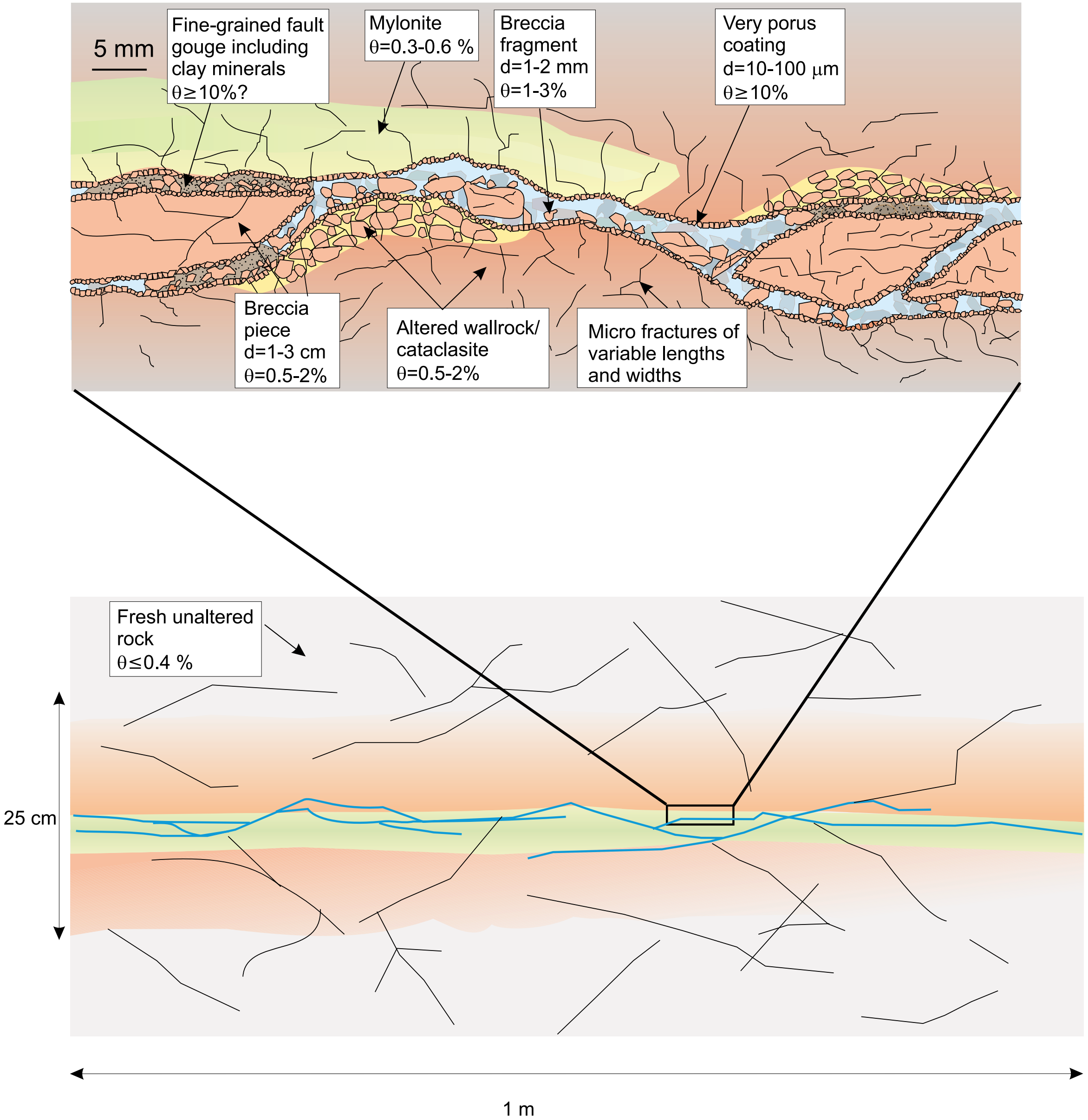


__Figure EX-2.__ Generalised conceptual model of a typical conductive structure involved in the tracer experiments. The lower part of the figure highlights the existence of a altered rim zone centred on a mylonitic precursor with cataclastic insertions. The number of conductive fractures may vary along the extent of the structure.

In situ tracer tests

Successful tracer experiments over longer distances require a well established hydraulic control and understanding. The key design challenge associated with tracer tests run on larger length scales was to select a test geometry that could produce reasonable mass recovery and the major portion of the breakthrough curve within a practical time frame. Early in the characterisation, tracer injections were run in conjunction with cross-hole interference tests to identify pathways meeting these requirements. Once feasibility was demonstrated, a more structured search for ideal source (injection) and sink (pumping) sections commenced. This search culminated during Phase A after which the prioritised sink section was selected. This phase also included tracer tests run with the objective to identify source sections for the subsequent tests with radioactive sorbing tracers. Phase B included tests to demonstrate sufficiently high mass recovery of conservative species to warrant use of radioactive tracers. For the final Phase C, four injections of cocktails of radioactive sorbing tracers were made in three different source-sink pairs over distances ranging between 15 and 100 m, as integrated along the structures of the hydrostructural model. Injection C1 being run essentially in a single structure flow path in Structure #20 (15 m) and C2 in a multi-structure flow path with a maximum length of 100 m. Flow path C3, originally interpreted as a single structure flow path in Structure #21, turned out to be a more complex flow path than originally anticipated. The tracer cocktails were administered either as decaying pulses, or near finite pulses, into a radially converging flow field. In some cases with a low injection flow rate in the source section producing a strongly unequal dipole (~1:50). The radioactive sorbing tracers used were mainly cations selected from the alkali and alkaline earth metal groups.

A total of 16 flow paths were tested, of which 50% represent interpreted single-structure flow paths and the remainder represent multiple-structure flow paths of variable complexity. Generally, the longer flow paths show low mass recoveries (< 60%), partly attributed to fracture intersection effects (connection to secondary sinks). All network flow paths show less steep tailings in log-log plots of the breakthrough curves for conservative tracers, compared to those observed in single structures, indicative of stronger diffusion effects. An example of breakthrough of sorbing tracers in the fast single-structure flow path I (Injections C1/C4) is shown in Figure EX-3. A breakthrough of the moderately to strongly sorbing tracers (Ba^{2+}, Rb^{+} and Cs^{+}) was not observed for injections C2 and C3 over the duration of the "official" monitoring period which ended November 2000. However, the sampling and analysis has continued through the end of 2002. The assembled tracer test data collected as part of TRUE Block Scale constitutes a unique database on *in situ* transport and retention in fractured crystalline rock over distances up to 100 m.

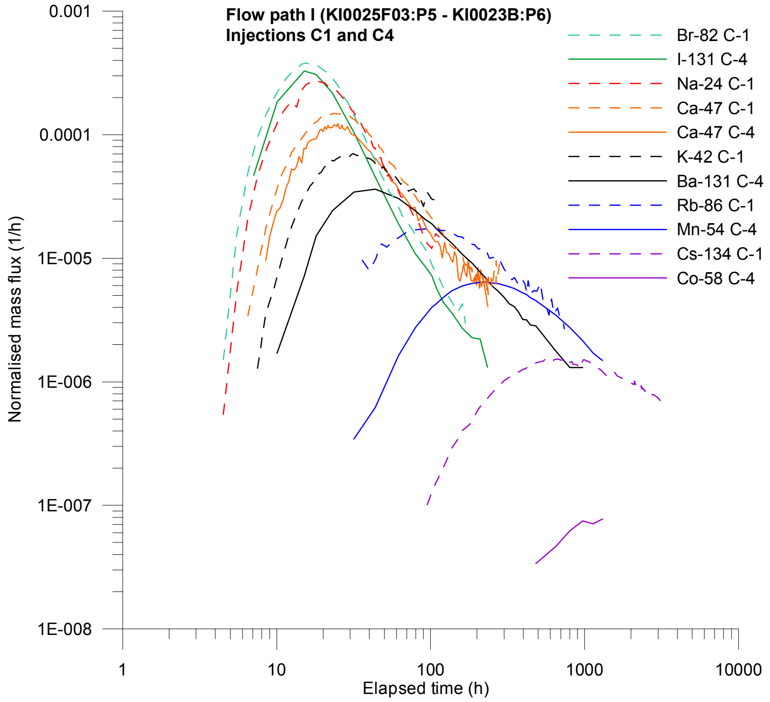


Figure EX-3. *Normalised tracer breakthrough for all tracers injected in tests C1 and C4.*

Modelling of flow, transport and retention

Numerical modelling has constituted an important and integrated component in the successful performance of the TRUE Block Scale Project. Early on in the project, modelling was restricted to Discrete Feature Network modelling (DFN). During the Detailed Characterisation stage Stochastic Continuum (SC) and Channel Network (DFN/CN) approaches were included. Modelling efforts culminated with the predictions and evaluations of the Phase C tracer tests, partly guided by the formulated hypotheses. This last phase of modelling included two additional concepts, the LaSAR concept and the Posiva streamtube approach.. The former three models were implemented in 3D and provided 3D solutions to the flow problem. Boundary conditions to these models were collected from available site-scale models. The latter two models made use of existing flow solutions or measured residence times obtained from conservative tracer tests (Phase B) to solve the transport problem. To the above five concepts should also be added the 1D advection-dispersion approach used for the basic evaluation of each tracer test.

A major accomplishment is the common conceptual basis for transport and retention which was developed within the project. The fractured crystalline rock volume is here conceptualised as a dual porosity (mobile-immobile) system where indivisible tracer particles (e.g. radionuclide ions) are transported through one or several fractures. The mobile pore space is primarily made up of the relatively small portion of the total pore space made up of the conductive fractures. Water in the remaining majority of the available pore space in the rock matrix and fracture filling material is effectively regarded as immobile. Tracer tests were designed to study both network effects in advective transport and mass transfer processes between the mobile and immobile pore spaces. Tracer particles are assumed to be subject to two processes: (i) advection due to water movement and (ii) retention in the rock matrix and on rock surfaces due to diffusion and sorption. In other words, retention processes retard particle movements relative to the flowing groundwater. It is noted that the main difference between the concepts/approaches lies in how heterogeneity is treated and the extent to which the various immobile zones are taken into account, and how they are implemented.

For predictions of the *in situ* radioactive sorbing tracer tests, the modelling groups were given access to the results of the cross-hole interference tests, tracer dilution tests and results of relevant non-sorbing tracer tests performed in the flow paths at relevant pump rates (from Phases A and B). They were then asked to predict the reactive tracer breakthrough and associated mass recovery of the Phase C tests and performance measures in terms of arrival times for 5%, 50% and 95% of the tracer mass and overall tracer mass recovery.

Address of the Basic question #1 included analysis of whether the developed hydrostructural model could be shown to properly account for the heterogeneity of the rock mass, whether it is consistent with observed patterns of connectivity, and finally, whether the hydrostructural model is consistent with the results of performed tracer tests. The overall finding from the analysis was that the hydrostructural framework overall is consistent with available *in situ* data. The ability of the evolving hydrostructural model to simulate tracer transport was also evaluated. It was shown that a numerical model based on the most recent hydrostructural model had a significantly better ability to reproduce selected tracer test results compared to a model based on the older, less mature hydrostructural models.

Address of Basic question #2 included analysis of whether effects of fracture intersection zones (FIZ) could be detected in available breakthrough curves and differentiated from effects of heterogeneity within individual planar structures.
It is noted that the constitution of FIZs in essence could resemble those of channels developed in fracture planes. This primarily attributed to the fact that FIZs most likely do not exhibit a clear-cut singular characteristic, but rather can show a combination of barrier and conductor characteristics. Modelling studies could not distinguish effects of fracture intersection zones on evaluated pathway transport parameters. However, it appears to be possible to distinguish FIZ effects in terms of tracer mass lost to alternative sinks along related pathways, if the FIZ is hydraulically connected to the secondary sink. A correlation was in this context noted between tracer mass loss and flow paths passing fracture intersection zones. However, the tests concerned are all associated with longer flow paths, such that connections to other alternative secondary sinks are plausible.

***In situ* retention in the block scale**

Tracer retention has been examined using a basic division in the following two sets of processes;

- Advection + equilibrium sorption.
- Matrix diffusion (kinetic) which is governed by a) the flow field geometry and b) the modelled immobile pore spaces and material retention parameters.

Depending on the model approach different weight may be put on the two blocks of processes.

Properties of the flow field are crucial for transport and have an important role in determining the retention properties, which are assigned to the different transport paths. Advection here denotes transport of an ideal non-sorbing and non-diffusive tracer through the mobile pore space. The advective flow field effectively determines the relative importance of the different retention processes. In a steady-state flow field, flow paths of the tracer particles coincide with the streamlines of the flow field. Advective transport is governed by the properties of these streamlines. Under steady state and purely advective flow conditions, the tracer molecules follow the streamlines of the flow field. This means that the residence times of the ideal non-retarded tracer molecules are those of the streamlines. This residence time distribution is also referred to as the “groundwater residence time distribution”. A comparison of the advective fields employed by the five modelling groups in the prediction and evaluation of the Phase C tracer experiments show different emphasis on spreading due to the flow field relative to that produced by the retention processes. In order to match *in situ* results, models that produce narrow peaks in the simulated non-reactive and non-diffusive Dirac breakthrough curves require retention models that produce more spreading than models that produce dispersed breakthrough already as a consequence of the advective field.

The flow field related properties that govern tracer can be assessed by integrating the available information on flow path volume (from transit time and injection flow rate) and the volume-based apertures and interpreted flow paths lengths. The parameter β which define the flow field geometry and effectively accounts for the water residence time per unit half-aperture, is depicted in Figure EX-4. Flow path I (C1) shows a consistent grouping of most of the models showing values between 20 to 60 h/mm. It is noted, that flow path I gave breakthrough for the largest number of tracers and thereby the constraining power of the breakthrough curves is highest for this flow path. The retention parameter β should increase with increasing path length which is also clearly visible in Figure 6-5 (estimated path lengths C1<C3<C2).

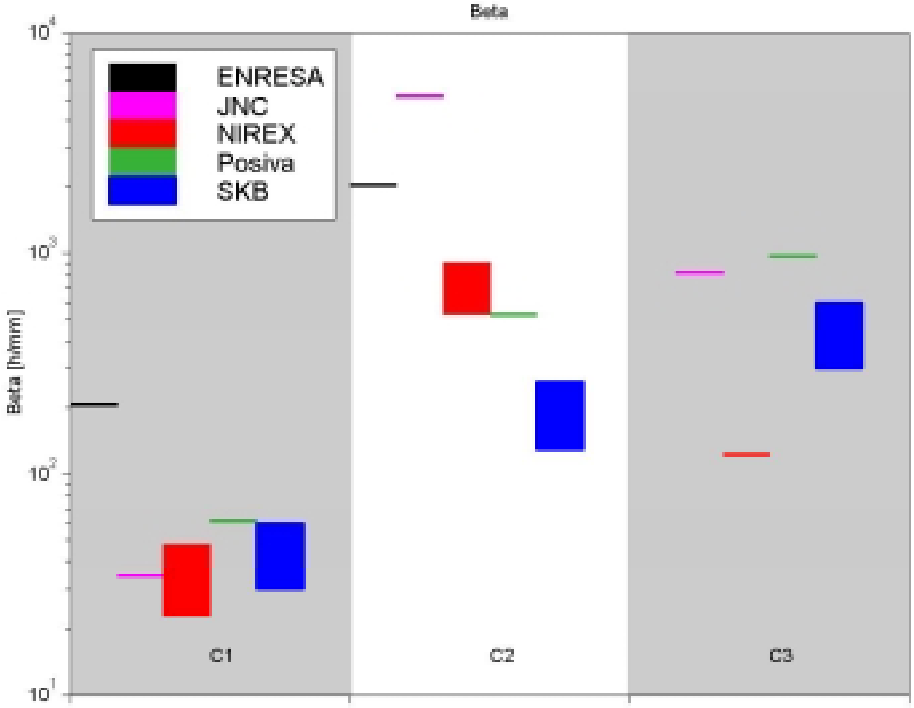


Figure EX-4. *Estimated flow path geometry β that describes the average flow geometry of the flow paths of the various models and flow paths (tracer tests).*

Diffusion to the immobile pore space, sorption in the immobile pore space and surface sorption on the fracture surfaces along the transport paths are interpreted to be the main retention processes in all prediction and evaluation models applied to the TRUE Block Scale experiments. This interpretation is supported both by the characteristics of *in situ* tracer test results and modelling where the measured residence time distributions can be reproduced more accurately with diffusional mass transfer invoked. Geological information from the TRUE Block Scale site supports the assumption of multiple immobile zones along the tested flow paths, cf Figure EX-2. The total volume of increased porosity (relative to that of the intact unaltered rock matrix), i.e. the retention capacity, is assumed small. The limited capacity may be an important factor for some of the immobile pore spaces e.g. stagnant pools, fault gouge and the altered rim zone. If a given immobile pore space becomes saturated it ceases to show kinetic diffusion mass transfer behaviour. In the case of fault gouge, the effects can then be modelled as being a part of the equilibrium surface sorption. The rock matrix has practically an infinite capacity in any *in situ* tracer experiment. Apart from the variable capacity of the pore spaces, the multiple and parallel appearance of the available immobile pore spaces causes superposition of similar response characteristics in the measured breakthrough curves. This means that it is not possible to unambiguously distinguish the contribution of diffusion to the different pore spaces using the breakthrough data alone.

Heterogeneity in the immobile zone properties influences the interpretation of *in situ* retention. Site-specific measurements indicate that the porosity immediately adjacent to the fracture surface is much higher than the average porosity of the intact unaltered rock. This high porosity zone adjacent to the fracture (including a very thin high-porosity coating) has significant impact on tracer retardation over experimental time scales. This difference in porosity may partly explain the noted differences between the retention observed in the laboratory and that observed *in situ*. Similarly, variability in porosity along the flow path implies larger "effective" porosity for retention than say the arithmetic mean porosity; this fact is also relevant for interpreting and understanding the observed enhanced retention.

Transport of selected tracers and radionuclides in crystalline bedrock is reactive. This means that the tracer particles interact with the groundwater-rock system by various chemical reactions during transport along the flow paths. In transport modelling, all these reactions, such as adsorption and ion exchange, are referred to as "sorption". Sorption may take place onto any geological material that is available along the studied transport path. Potential sorption sites along the flow paths investigated in the TRUE Block Scale experiments are located in and along the available mobile and immobile pore spaces.

The sorption models that have been applied by the modelling groups in the analysis of the TRUE Block Scale tracer experiments are based on simplified representations of the natural system. All models employ reversible and instantaneous equilibrium sorption. Fixed distribution coefficients, K_d, or K_a, are used to parameterise sorption of the different tracers. The latter two parameters depend only on the tracer used, the geological material and the groundwater composition. Depending on the modelling approach, the applied sorption values are based either on the fitting of breakthrough curves from previous *in situ* experiments at Äspö HRL and/or laboratory measurements that have been interpreted using the K_d approach. The sorption capacity of the fault gouge material is based on estimates of K_d derived from i.a. site specific mineralogy and groundwater composition.

Tracer retardation depends on the integrated (effective) retention property along the flow paths. This integrated property is composed of the porosity and pore diffusivity of the immobile zones paired with the sorption properties of the tracer and the properties of the flow field. It is not possible to evaluate the individual physical *in situ* retention parameters, or at least not in a unique way without additional independent information. The interpretation of the retention properties from the breakthrough curves is also strongly linked to the underlying assumptions related to of the advective flow field and equilibrium surface sorption. Figure EX-5 shows the integrated immobile zone parameter group κ associated with individual tracers used by the modelling groups in their evaluation modelling of the Phase C tracer tests. The large spread in the applied values of immobile zone properties indicates the embedded uncertainty. The majority of values applied are higher than values associated with intact unaltered wall rock (the so-called MIDS data set, cf /Winberg et al, 2000/).

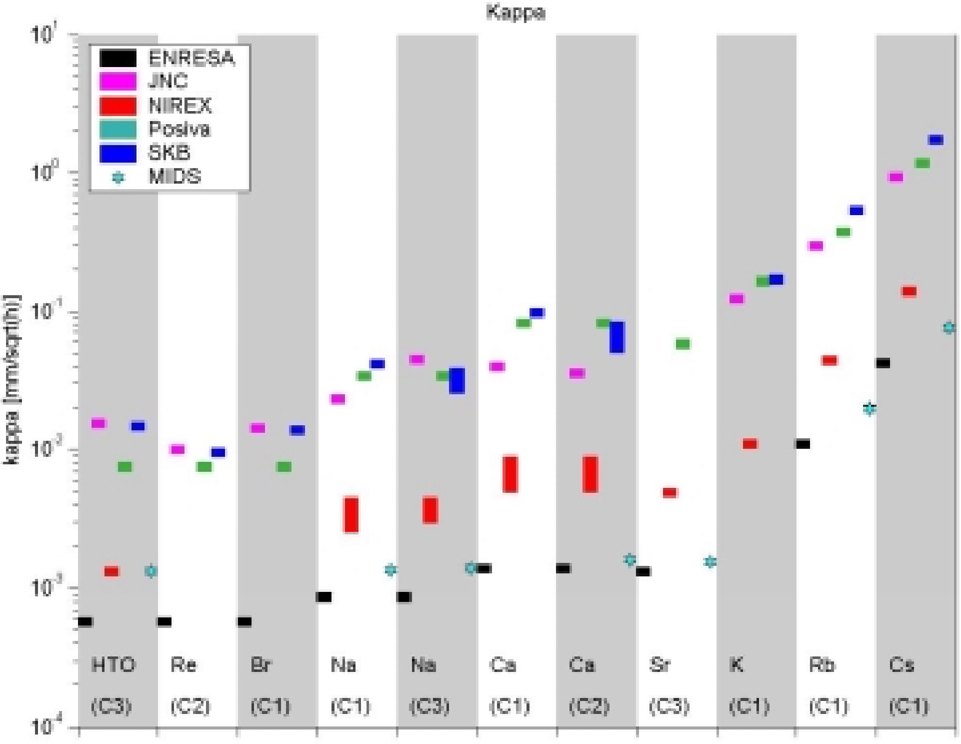


Figure EX-5. *Values of evaluated retention material parameter group* $\kappa=\theta\,(D(1+K_d\,\rho/\theta))^{1/2}$ *for the respective evaluation models and tests (C1, C2 and C3).*

Summary of *in situ* retention as seen in the TRUE Block Scale tracer tests

The experimental and modelling work associated with the TRUE Block Scale tracer experiments have achieved the following principal findings and results:

- It is demonstrated that the applied transport modelling approaches share the same basic theoretical basis. The difference between the approaches lies in how heterogeneity is introduced and parameterised.

- The observed *in situ* retention cannot be explained by surface sorption alone.

- All modelling groups assign matrix diffusion as an important, if not dominant retention mechanism. The existence of diffusional process is also evidenced by characteristics of the measured breakthrough curves.

- Geological evidence indicates that other immobile pore spaces than the wall rock matrix are likely to exist along the studied TRUE Block Scale flow paths (e.g. fault gouge/fault breccia and stagnant zones).

- Porosity is significantly higher in the thin, peripheral layer of the altered fracture rim zone, and it decreases normal to the fracture to attain a background value of the intact unaltered rock several millimetres to a few centimetres away.

- Retention is governed by parameter groups (involving flow field, immobile zone diffusion properties and sorption). It is found difficult to fully discriminate between the basic retention processes and come up with unambiguous *in situ* values on retention parameters without additional constraints.

- Heterogeneity in retention properties of the immobile zone may have important influence on the interpretation of *in situ* test results. Possibly most important is heterogeneity normal to the fracture surfaces (effect on kinetics, effective properties). Inclusion of heterogeneity in retention parameters may provide partial explanation of differences between predictions based on laboratory retention data and *in situ* measurements.

- The observed *in situ* retention of the TRUE Block Scale flow paths is similar to that observed in the flow paths investigated as part of the detailed scale TRUE-1 experiments.

- No additional phenomena/processes were required to explain the block scale test results. The same basic model used for single structures, as applied to the detailed scale TRUE-1 experiments, is also applicable also to a network of structures (attributed to the integrating nature of matrix diffusion process).

Major accomplishments

- **Useful toolkits for site characterisation**
  The TRUE Block Scale Project has confirmed the value of a number of powerful but uncomplicated characterisation techniques. Posiva flow logs identify the conducting intervals in boreholes with a high resolution. BIPS borehole imaging and BOREMAP core logging provide geologic descriptions of the conductors. Single-hole transient tests produce reliable information on hydraulic properties. Pressure monitoring during drilling and hydraulic testing indicates the connectivity along conductive features within the borehole array. Additional information from long-term pressure monitoring, hydrogeochemical sampling of groundwater, and background groundwater flow, provide a basis for conceptualising the flow system in the studied rock volume. It is noted that hydrochemical data provide support for a partly compartmentalised system.

- **Integrated network characterisation methods provide an adequate hydrostructural descriptive model in support of block scale experiments**
  Within the limitations imposed by the underground openings and possible collar positions for drilling, the borehole array provided an acceptable basis for establishing the hydrostructural model of the studied rock volume. The geological, geophysical, hydrogeological and hydrochemical investigations have provided a satisfactory and mutually supporting basis for the *in situ* experimentation.

- **Improved description of porosity and porosity distribution**
The laboratory data provided new insight into the heterogeneous nature of the studied flow paths. Improved understanding has been gained about the porosity characteristics of selected constituents of fault rock zones. Similarly, additional support has been presented regarding the decreasing trend in porosity normal to the fracture surfaces, observed already in conjunction with TRUE-1.

- **Improved microstructure conceptual models of conductive structures/fractures**
Conceptual models for conductive fractures in fractured crystalline rock have been significantly improved through the work performed within the scope of the Fracture Characterisation and Classification Project (FCC) and TRUE programs at Äspö. Although the conceptual components are relatively well defined, it is yet to fully parameterise some of its constituents (such as porosity/diffusivity of fine-grained fault gouge).

- **Simplified description of far-field from a performance assessment perspective**
The results of the TRUE Block Scale experiments, thus far, do not require additional processes or features relevant to the safety case, which were not known from previous experience from TRUE-1. In addition, the results from tests with sorbing tracers, run over projected length scales 15–100 m, have shown similar retention to what was observed at the TRUE-1 site (5 m length scale). This finding, although of limited statistical significance, may indicate that complicated spatial scaling or parameters when taking limited steps in space is not important. It should in this context be noted that the effects of temporal scaling when taking the step from experimental to performance assessment time scales may not be that easy to assess.

- **Identification of retention data needs for repository site characterisation**
Over the practical time frames of *in situ* experimentation, the retentive capacity provided by the near proximity rock adjacent to conductive fractures/flow paths will be involved in the retention of tracers. This combined with the defined parameter groups accounting for the individual retention processes, calls for improved laboratory quantification of diffusivity, porosity and sorption. It should, however, be emphasised, that a laboratory programme will never account for the exact mix of properties which the tracers will experience along a given flow path. Effectively we are only in a position to assess the situation at the source and at the sink. Exhaustive laboratory tests and statistical inference can in principle resolve this problem of uncertainty, but there is no guarantee to fully understand the particular flow path. In essence, we know the integrated response of a given flow path and our job is, to the best of our ability, to narrow down and constrain the *in situ* parameter estimates.

  In the perspective of site characterisation for a geological repository, and subsequent performance assessment, the situation is different. Over the time span of a geological repository the retentive capacity of the close proximity rock (altered rim zones, fault breccia/fault gouge) will be consumed relatively quickly. This implies that the retentive capacity of the intervening rock blocks can be viewed as essentially infinite. However, this assumption is very much dependent on the extent of the connected porosity beyond the altered rim zone. At present, firm proof of infinite capacity is not available.

- **Inherent limitations in site characterisation with regards to collection of data relevant to PA**
  The methodology employed in TRUE Block Scale does not provide a direct means to assess the flow-field controlled contribution to retention through parameters like β (or 2WL/q), cf Section 5.5, from site characterisation data alone. The parameter 2WL/q can however be estimated one the basis of geometrical inferences paired with flow data, the latter either from borehole flow data (ambient flow rate from tracer dilution tests) or from modelling. Alternatively the parameter β can be estimated using model simulation.

- **Evaluation of conservative assumptions**
  The improved conceptualisation and parameterisation of fracture rim zones and infillings can add additional, although limited, margin to safety. This applies especially to those radionuclides, which are expected to be permanently fixated by clay minerals associated with the altered rim zones.

Contents

1 Introduction

1.1 Organisation of report

The current report which constitutes volume 4 out of four in the TRUE Block Scale Final Report series serves two different purposes. First, this report conveys in a condensed fashion the important results from the characterisation, *in situ* testing and the numerical modelling. Second, this report provides a synthesis of the current understanding of flow, transport and retention in fractured crystalline rock at the block scale.

Chapter 1 provides background, rationale and objectives of the project and also provides an overview of the scientific understanding in an international perspective. Further the questions asked prior to onset of the *in situ* tracer tests and hypotheses posed are presented.

Chapter 2 describes methodology and experience gained in the identification of conductive fractures and hydraulic connectivity in fracture networks. In addition the construction of hydrostructural models and conceptual flow models and their bases are discussed. Furthermore, the applications of the project's methodologies to repository site characterisation and development are discussed.

Chapter 3 provides an overview of laboratory-related accomplishments including formulation of a generalised detailed conceptual model of target structures and their immediate surroundings.

Chapter 4 accounts for findings and accomplishments of the *in situ* tracer tests with discussion of differences between single structure and network flow paths, and comparison with TRUE-1 results.

Chapter 5 presents the results of the numerical modelling with special emphasis on addressing the defined hypotheses. A common conceptual basis for transport modelling is presented as well as an assessment of the relative effects of different transport and retention processes.

Chapter 6 provides a compilation and discussion of major project accomplishments with special emphasis on site characterisation and performance assessment associated with a geological repository.

Chapter 7 gives an overview of ongoing and planned research associated with the TRUE-1 Continuation and TRUE Block Scale Continuation projects.

1.2 Background

Concepts for the deep geological disposal of spent nuclear fuel include multi-barrier systems for isolation of nuclear waste from the biosphere. Waste forms, and concepts for encapsulation of the waste and engineered barriers may vary between countries, but most concepts rely on a natural geological barrier which should provide a stable mechanical and chemical environment for the engineered barriers, and should also reduce and retard transport of radionuclides released from the engineered barriers. In case of an early canister failure, the retention capacity of the host rock in relation to short-lived radionuclides such as Cs and Sr become important.

In planning the experiments to be performed during the Operating Phase of the Äspö Hard Rock Laboratory, the Swedish Nuclear Fuel and Waste Management Company (SKB) identified the need for a better understanding of radionuclide transport and retention processes in fractured crystalline rock. This understanding is a cornerstone of performance and safety assessments of the natural barrier system and it has three essential parts:

- Demonstrating the ability of numerical models to simulate transport processes involving sorbing radionuclides.
- Showing that field experiments involving practical site characterisation tools could identify pathways and obtain the *in situ* transport/retention data needed to characterise the flow paths through numerical simulations (e.g. in terms of distribution coefficients, diffusion parameters and flow-related properties that govern *in situ* retention.
- Identifying approaches for integrating laboratory data on transport parameters with field-scale results at variable length scales.

To answer these needs, SKB in 1994 initiated a tracer test programme named the Tracer Retention Understanding Experiments (TRUE). The objectives of TRUE are given in Section 1.4.

The First Stage of TRUE (TRUE-1) was performed in the detailed scale (0–10 m) and was focused on characterisation, experimentation and modelling of an interpreted single conductive feature /Winberg et al, 2000/. The programme involved the staged drilling of five boreholes, site characterisation, and installation of multi-packer systems to isolate individual water-conducting features. Subsequent cross-hole hydraulic tests and a comprehensive series of tracer tests were used to plan a series of three tracer tests with radioactive sorbing tracers. The *in situ* tests were supported by a comprehensive laboratory programme performed on generic as well as on site-specific material from the studied feature. In addition techniques for characterisation of the pore space of the investigated flow paths using epoxy resin were developed and successfully tested *in situ*.

The various phases of the tracer tests performed as part of TRUE-1 were subject to blind model predictions and subsequent evaluation /Elert, 1999; Elert and Svensson, 2001; Marschall and Elert, in prep/. The results of the TRUE-1 experiments showed clear evidence that diffusion processes affect transport. The experiment left unresolved, however, whether the diffusion was occurring dominantly in the wall rock of the flowing features or if diffusion was confined to a damage-zone of fault gouge and similar fine-grained material within the conductors themselves. This issue is central to determining how much of the rock mass volume that participates in retention processes and ultimately governing the retention capacity of the natural barrier system. A major feature of the TRUE-1 programme was the development of resin-injection methods to help resolve this issue.

The original conceptualisation of the TRUE program recognised that transport is not confined to a single feature in nature. Rather, transport in natural systems involves networks of conductive features where solutes must pass through intersections, and diffusion occurs in rock blocks bounded by conductors. Questions persisted regarding the effects of a fracture network and its components on transport and retention. Accordingly, the original TRUE plans called for a block scale experiment involving multiple conducting features that would complement the findings of the TRUE-1 programme. The programme defined "block scale" as involving multiple conductors and pathways of tens to a hundred or so meters in length. Accordingly, this experimental programme was initiated as the TRUE Block Scale Project. This report, which is the last in a series of four volumes, summarises the main findings from the TRUE Block Scale Project and provides a synthesis of understanding of block scale flow, transport and retention in fractured crystalline rock.

1.3 Rationale

1.3.1 Performance assessment

The block scale is the critical region of the natural barrier system in the performance assessment approaches of many international programs. Major conducting features, such as those that produce lineaments on the ground surface or create geophysical anomalies, have spacings that are at the same scale or larger than the block scale, that is, greater than a hundred metres. Although these major conducting features may have retentive properties, some views of performance assessment look for the major portion of the natural barrier performance to occur in the region between waste emplacement sites and the major conducting features.

Understanding flow and tracer transport at the scale between that of a single fracture, which might intersect a disposal canister position, and the major conducting features is precisely the block scale of interest for the TRUE Block Scale program. This understanding focuses on the geology and 3D geometry of the conducting features and how this geology controls the retention characteristics of the rock mass, both from a physical standpoint (distributions of flow rate, porosity and flow-related transport properties) and chemical standpoint (mineralogy and geochemistry of materials lining fractures surfaces and pore spaces and the geochemistry of the groundwater). The block scale differs from the single-fracture emphasis of the TRUE-1 experiments in expanding these concerns to multiple fractures and the their network geometries including possible additional effects in fracture intersections.

1.3.2 Site characterisation and repository development

The block scale is also important from the perspective of selecting and developing repository sites. The site selection process may need to include block-scale performance as a screening consideration. However, detailed characterisation of block-scale behaviours would not be likely until repository sites are developed underground. One objective of underground test facilities such as the Äspö Hard Rock Laboratory is to have well-characterised sites for comparison with candidate repository sites that will likely not be as thoroughly characterised at the time of site selection. The data collected in the block scale, whether obtained from the surface or from underground openings, are also important for the development of the detailed layout and design of a repository. Block scale data can be used to develop criteria for offsets (safety distances) of disposal locations (storage tunnels and canister positions) from conducting features, as well as providing geohydrologic bases for determining the density of waste-package emplacements.

An experiment on the block scale hence provides a training ground for developing tools and methodologies to be employed primarily in future detailed characterisation for a geological repository, and as support for models and concepts utilised in performance assessments.

1.3.3 Modelling

Block scale (10–100 m) description of flow and transport provides opportunity for application of a variety of different modelling approaches and evaluation relative to available experimental results. Among the 3D approaches (which can provide description of both flow and transport in low-permeable crystalline rocks) are stochastic continuum (SC), discrete feature network (DFN) modelling and channel network modelling (DFN/CN). Interesting questions arise at this particular scale. Depending on the problem at hand and the type of heterogeneity seen in the rock, can a smallest scale be identified at which the stochastic continuum approach can resolve flow and transport phenomena? Is it necessary to use discrete approaches below this threshold length scale to account for needs to incorporate and account for a higher degree of complexity/heterogeneity?

At the same time, the block scale constitutes a challenge for the more performance assessment related modelling approaches such as the LaSAR and Posiva streamtube approaches. Despite the simplification of the natural system employed in the TRUE Block Scale modelling; do the models provide adequate descriptions of flow and transport and are the model results adequate?

One of the basic ideas embedded in the TRUE Programme is that experimentation at various scales – laboratory (< 0.5 m), detailed scale (< 10 m) and block scale (10–100 m) – will provide a basis for improved understanding on how to simulate numerically flow and transport, and how to link transport models and transport parameters at different scales. A major goal of the TRUE experimental programme is to reduce the uncertainties associated with extrapolation and prediction on a site scale (0.1–1 km). The TRUE Block Scale experiment here constitutes the higher end member of the studied experimental scales.

1.3.4 Transport and retention

The principal differences between the TRUE-1 and TRUE Block Scale experiments include the larger spatial scale of the experimentation and the inclusion of multiple conducting features along the transport pathways. Of principal interest is whether the longer transport distances in themselves, through a higher degree of heterogeneity, will provide exposure to larger surface area, and thus more retention.

In addition, the performance of tracer tests in a network of structures may investigate whether or not fracture intersection zones (FIZ) are regions with distinctive flow and transport properties that influence tracer movements. Although TRUE Block Scale does not provide an experimental array with the specific aim to investigate FIZs, the results from the experiments may still provide indirect evidence of the possible effects of FIZs. In TRUE Block Scale, the tracer test pathways were evenly divided between single structure pathways and multiple-feature pathways /Andersson et al, 2002b/, in the latter case where transport flow paths had to cross fracture intersection zones.

The results from the TRUE-1 experiments /Winberg et al, 2000/ used radioactive tracers that varied in their sorptive behaviour. These tracers were (in order from lowest sorptivity); $Na^+ < Ca^{2+} \approx Sr^{2+} << Rb^+ \approx Ba^{2+} < Cs^+$. The ranking of the sorptive behaviour for these tracers was consistent for both laboratory and *in situ* tests. The TRUE Block Scale programme investigated whether or not this ranking of sorptive behaviour could be extended to a larger scale than previously tested.

Explicit evidence for the existence of gouge material (fault breccia/fine-grained fault gouge) has not been found in Feature A investigated at the TRUE-1 site /Winberg et al, 2000/. Modelling performed within the Äspö Task Force has shown that assumptions of a geologic material with increased porosity/sorptivity in direct contact with the flowing groundwater, e.g. gouge material, can explain the observed increased retention in TRUE-1. Fault gouge can be very fragile and difficult to recover, even when using sophisticated triple-tube coring. In the network of structures investigated as part of TRUE Block Scale, however, there is a firm evidence of fault breccia and fault gouge from the core logging, cf /Andersson et al, 2002a/. Estimates of fault gouge sorption properties, with all due respect to uncertainties about the distribution of fault gouge material along a flow path, are expected to provide means for improving the understanding of the relative contribution to retention from the rock matrix and fault gouge material, respectively.

1.4 Scientific understanding at onset

1.4.1 Relevant experimental and modelling results

During the past 25 years significant efforts have been made world-wide to improve understanding of fractured crystalline media as host rock for a geological repository. This development has included fieldwork at various test sites and underground laboratories in a number or countries. In parallel with the field activities have been international exercises in cross-verification of numerical methods (INTRACOIN, HYDROCOIN, INTRAVAL) which have used the results of the underground laboratory experiments for some of their test cases. INTRAVAL was followed by GEOTRAP that provided a platform for discussion of issues related to understanding and modelling radionuclide migration.

For the most part the characterisation work, field experiments and subsequent modelling during this period have focused on conceptualisation of groundwater flow with particular emphasis on different approaches to incorporate and describe the heterogeneity of fractured rock. This includes the extension of homogeneous continuum models to stochastic continuum models (SC). Here the position and geometry of fractures and fracture zones are included as tessellated continuum blocks with properties other than in the rock mass blocks in between. Another approach to describing heterogeneity has been the discrete feature network model approach (DFN) where existing fractures are included explicitly usually as circular or ellipsoidal shapes. The size, frequency/density and material properties can be sampled from statistical distributions parameterised from site characterisation data. A further refinement of the DFN approach is the channel network model (DFN/CN) where a fracture network model is reduced to equivalent pipe-network connections. These pipes may be either single conduits that represent the connection between two fractures, or they may be pipe networks lying within the fracture planes that mimic the channelisation due to heterogeneity within a fracture plane, cf Figure 1-1.

The development of new numerical approaches has also triggered development of *in situ* characterisation techniques to map fractures at depth. These techniques include various seismic techniques including cross-hole applications. Similarly, borehole radar techniques were developed including directional antenna by which the geometry of fractures could be assessed. The development of site characterisation technologies has had a mutually stimulating effect with transport conceptualisation and numerical modelling. Conceptualisations of transport inspire new methods of characterising rock masses, and the results of new characterisation approaches provide new insights into the conceptualisation and transport processes both for the conducting pathways and the intervening rock blocks. Development of geostatistical methods and geostatistical simulation tools for flow and transport today also allow for usage of soft information (e.g. lithology and geophysical data). Some geostatistical techniques also incorporate inverse techniques, which also can make use of state variables like hydraulic head.

In the area of transport and retention *in situ* experimentation has been relatively scarce, and, with a few exceptions, mainly focused on conservative (non-reactive) transport experiments over relatively short distances.

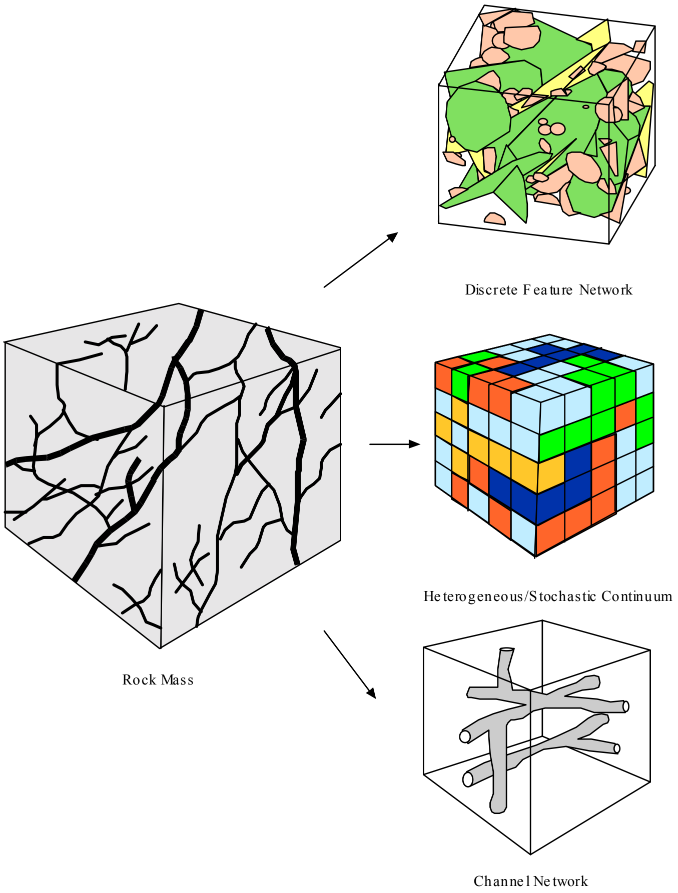


Figure 1-1. Overview of different model approaches to fractured crystalline rock.

In **Sweden** experimentation in groundwater flow and radionuclide transport began in 1977 with the Stripa Project, carried out in the abandoned iron ore mine in central Sweden /e.g. Fairhurst et al, 1993/, and surface-based work at the Finnsjön test site /Andersson, 1993/. At both these sites tracer experiments were conducted at various scales and using on-reactive and sorbing tracers. At Stripa transport experiments /Birgersson et al, 1992/ were performed on single fractures (Phase I), fracture zones (Phase III) and in 3D fracture networks in a near fracture environment (Phase II). The main conclusions related to Phases I and II /Fairhurst et al, 1993/ were the following:

- “The existence of channels in natural fractures seriously complicates the analysis of tracer transport data. It is difficult to identify the mechanisms of nuclide retardation and to quantify the path lengths and the dispersivity characteristics”.
- “The characteristics of the groundwater flow field and the migration pathways in a volume of rock must be carefully quantified before conducting an *in situ* tracer test. This level of understanding is necessary in order to analyse properly the tracer test data”.

For Phase III of the Stripa Project (1988–1992) a considerable effort was placed on defining the geometry and flow characteristics of the H fracture zone in the SCV site using radar and hydraulic testing before initiating the tracer experiment in that zone /Fairhurst et al, 1993/.

During recent years tracer experiments have been conducted at the Äspö Hard Rock Laboratory. A large-scale tracer experiment was performed as part of the LPT-2 pumping test during which conservative dye and radioactive tracers were administered to borehole sections distributed around the pumped section. The experiment was subject to modelling as part of Task 1 of the Äspö Task Force work /Gustafson and Ström, 1995/. Within the TRUE programme experiments being part of TRUE-1 were focused on an interpreted single fracture at distance from the access tunnel where experiments with conservative and sorbing tracers were conducted over a 5–10 m length scale, cf Section 1.3.2.

Similar block scale site characterisation has been performed in **Spain** (El Berrocal), **Switzerland** (BK site at the Grimsel laboratory), **Japan** (Kamaishi mine) and in **Canada** (URL, Whiteshell). The TRUE Block Scale Project has in particular benefited from the Kamaishi experience with regards to the usage of pressure responses due to drilling.

With regards to the solute tracer experiments, the TRUE Block Scale Project has foremost benefited from the experience gained from the Stripa Phase II work and the experiments with radioactive sorbing tracers at the Finnsjön site (Zone 2), at Grimsel MI /Smith et al, 2001/ and the TRUE-1 site /Winberg et al, 2000/.

1.4.2 Main findings from TRUE-1

Of particular significance to the TRUE Block Scale Project are the results of TRUE-1 performed at the Äspö HRL. TRUE-1 adapted tracer testing methods that were developed for surface-based investigations to the higher pressure and higher salinity encountered underground at Äspö HRL. In addition, the *in situ* tests with sorbing tracers at Äspö have produced calibrated retention parameters (or parameter groups) which, given the geological similarities between the TRUE-1 and TRUE Block Scale sites, provide a basis for predicting the results of the TRUE Block Scale *in situ* tracer tests.

The first stage of the Tracer Retention Understanding Experiments (TRUE-1) /Winberg et al, 2000/ was performed as an SKB funded project. The project collected *in situ* retention data from a series of cross-hole tracer tests, evaluated the usefulness and feasibility of different model approaches and provided a baseline for continued *in situ* radionuclide migration and retention studies at Äspö HRL. The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes coordinated the application of different modelling approaches for numerical simulation of the experiments. The TRUE programme has progressed by three stages with increasing scales of investigation: laboratory scale (< 0.5 m), detailed scale (< 10 m), and block scale (10–100 m). TRUE-1 addressed the detailed scale with the specific objectives of providing data and conceptualising a single feature. The tracer tests, which used both conservative and sorbing tracers, are to be followed by a future resin injection and excavation of the fracture to allow direct observation of the aperture and pore-volume distribution within and adjacent to the fracture.

The site for the TRUE-1 experiments is located at approximately 400 m depth in the northeastern part of the Äspö Hard Rock Laboratory. The identification of conductive fractures and the target feature benefited from the use of BIPS borehole TV imaging combined with detailed flow logging. The assessment of the conductive geometry was further sustained by cross-hole pressure interference data. The target feature (Feature A) is a reactivated mylonite, which has later undergone brittle deformation. The feature is oriented northwest, along the principal horizontal stress orientation, and constitutes a typical conductor for Äspö conditions. Hydraulic characterisation showed that the feature is relatively well isolated from its surroundings. The near proximity of the experimental array to the tunnel (10–15 m) implies a strong hydraulic gradient (approximately 10%) in the structure, which had to be overcome and controlled during the experiments.

The conservative tracer tests in Feature A showed that the feature is connected between its interpreted intercepts in the array. The parameters evaluated from the conservative tests – flow porosity, dispersivity and fracture conductivity – are similar, indicating a degree of in-plane homogeneity.

The *in situ* tracer tests, using essentially the same selection of sorbing tracers as in the laboratory were found to show the same relative sorbtivities as seen in the laboratory tests ($Na^+ < Ca^{2+} \approx Sr^{2+} << Rb^+ \approx Ba^{2+} < Cs^+$). A test using $^{137}Cs^+$ showed that approximately 60% of the injected activity remained sorbed in the rock after termination of the test (after some 11 000 hours).

The interpretation of the *in situ* tests with sorbing tracers performed by the project team was conducted using the LaSAR approach /Cvetkovic et al, 2000/, developed as a part of the TRUE project. In this approach the studied flow path is viewed as a part of an open fracture. Key processes are spatially variable advection and mass transfer. The evaluation showed that laboratory diffusion data are not representative for *in situ* conditions. A close fit between field and modelled breakthrough is obtained only when the parameter group which includes diffusion/sorption ($k \cdot \kappa$, cf Section 5.5) is enhanced with a factor varying between 32–50 for all tracers and experiments (except for Cs) and 140 for Cs^+. The interpretation is that the enhancement is mainly due to higher diffusivity/porosity and higher sorption in the part of the altered rim zone of the feature which is accessible over the time scales of the *in situ* experiments, compared to data obtained from core samples in the laboratory. Estimates of *in situ* values of the important transport parameters are provided under an assumption of a valid range of porosity in the accessible part of the rim zone in the order of 2–2.4%.

The TRUE-1 experiments produced results on the relative contributions to sorption of matrix pore surfaces, fracture surfaces, fracture gouge, at least for the time scales investigated by the experiment. The dominant retention sites were interpreted to be part of the rock matrix. The effects on tracer retention by equilibrium surface sorption and sorption in gouge material were found to be observable, but of secondary importance. Similarly, the effect of diffusion/sorption into stagnant water zones was found to be limited.

Alternative conceptualisations and interpretations of the experiments were performed as part of the work in the Äspö Task Force. An overview of the alternative interpretations of the TRUE-1 experiments is provided by /Elert, 1999; Elert and Svensson, 2001; Marschall and Elert, in prep/ and in /SKB, 2001/. Interpretations attributing the bulk of the retention to matrix diffusion effects associated with multiple flow paths and fault gouge /Mazurek et al, 2002; Jakob et al, 2002/ and 3D effects /Neretnieks, 2002/ have been proposed, respectively.

1.5 Objectives

The **overall objectives** of the Tracer Retention Understanding Experiments (TRUE) are to:

- develop an understanding of radionuclide migration and retention in fractured crystalline rock,
- evaluate to what extent concepts used in models are based on realistic descriptions of a rock volume and if adequate data can be collected in site characterisation,
- evaluate the usefulness and feasibility of different approaches to model radionuclide migration and retention,
- provide *in situ* data on radionuclide migration and retention.

The **specific objectives** of the TRUE Block Scale Project given in the developed test plan /Winberg, 1997/ are to:

1. increase understanding of tracer transport in a fracture network and improve predictive capabilities,
2. assess the importance of tracer retention mechanisms (diffusion and sorption) in a fracture network,
3. assess the link between flow and transport data as a means for predicting transport phenomena.

1.6 Overview of project

The TRUE Block Scale project is an **international partnership** funded by ANDRA (France), ENRESA (Spain), JNC (Japan), Nirex (UK), Posiva (Finland) and SKB (Sweden) /Winberg, 1997/. The Block Scale project constitutes one part of the Tracer Retention Understanding Experiments (TRUE) conducted at the Äspö Hard Rock Laboratory. The project, which was initiated mid 1996, is divided into a **series of defined stages**;

- Scoping Stage.
- Preliminary Characterisation Stage.
- Detailed Characterisation Stage.
- Tracer Test Stage.
- Evaluation and Reporting Stage.

The staged approach also has an embedded **iterative approach to characterisation** and hydrostructural modelling, whereby the results of the characterisation of each drilled borehole has been used to plan the subsequent borehole.

At the conclusion of the Detailed Characterisation Stage in mid 1999, the **feasibility of performing tracer tests** in the identified network of structures in the block scale (10–100 m) had been firmly demonstrated /Winberg, 2000/. Consequently, a series of tests with **radioactive sorbing tracers** were performed as part of the Tracer Test Stage, which ran from mid 1999 through 2000. Updates of the hydrostructural model after each borehole and each programme stage provided bases for modifying numerical models that predicted the results of the next round of drilling, hydraulic testing, and tracer tests. The **numerical model analysis** has been performed with **various modelling approaches**.

In support of the *in situ* experimentation, a series of **laboratory investigations** have been performed on geological material from the interpreted structures, which make up the studied fracture network. The analyses included mineralogical and geochemical analyses, porosity determinations using water absorption and PMMA techniques.
In addition, water samples collected during drilling and from packed off piezometer sections have been analysed for chemical composition and isotope content and used in support of the hydrostructural models. Cation-exchange capacity values for fault breccia material from different structures were, deduced from mineralogical composition. These exchange capacity values then have been used in combination with selectivity coefficient, mineralogy and ambient groundwater chemistry from the different test sections to estimate volumetric distribution coefficients (K_d).

1.7 Questions asked and tested hypotheses

The TRUE Block-Scale programme was framed as a set of experiments designed to address well-defined questions. Three basic questions have been posed in relation to the tracer tests /Winberg, 2000/, their planning, and their evaluation. These are:

Q1) “What is the **conductive geometry** of the defined target volume for tracer tests within the TRUE Block Scale rock volume? Does the most recent structural model reflect this geometry with sufficient accuracy to allow **design and interpretation of** the planned **tracer tests**?”

Q2) “What are the **properties** of fractures and fracture zones **that control transport** in fracture networks?”

Q3) “Is there a **discriminating difference** between breakthrough of sorbing tracers in a detailed scale **single fracture**, as opposed to that observed in a **fracture network** in the block scale?”

On the basis of these questions **corresponding hypotheses** have been formulated /Winberg, 2000/, to be **addressed by** the **tracer tests and** the **subsequent numerical analyses**;

H1) “The major conducting structures of the target volume for tracer tests in the TRUE Block Scale rock volume trend northwest and are subvertical. Being subvertical, and subparallel, they do not form a conductive network in the designated target volume. For the purpose of testing fracture network flow and transport effects in the current borehole array, second-order NNW features are required to provide the necessary connectivity between the major conducting NW structures!”

H2a) “Fracture intersections have distinctive properties and have a measurable influence on transport in fracture/feature networks. These distinctive properties may make the intersection a preferential conductor, a barrier, or a combination of both!”

H2b) “In-plane heterogeneity and anisotropy have a measurable influence on transport of solutes in a block scale fracture network!”

H3) “It is not possible to discriminate between breakthrough curves of sorbing tracers in a single fracture from those obtained in a network of fractures!”

2 Major findings from characterisation and building of hydrostructural models

2.1 Introduction

The TRUE Block Scale project used an **iterative characterisation strategy** from the beginning of the project. For every borehole, there was a prediction of what would be encountered. The results of drilling and testing were incorporated into an updated conceptual model of the block. An evaluation of the remaining uncertainties in the conductor geometries provided a decision basis for subsequent drilling and testing. The characterisation work spanned nearly five years (1996–2000). During this time characterisation methodologies also evolved. One evolution involved improvements in flow logging to identify conductive features in boreholes. Another development was closer integration of single-hole and cross-hole hydraulic testing.

Within the TRUE Block Scale Project it has been found that **identification and interpretation** of location/geometry and connectivity of **conductive structures** must use both geologic data and hydraulic data in a closely integrated manner. Geologic data and hydraulic data provide important mutual constraints on the conditions that exist within the studied rock volume. Not all geologic features have hydraulic importance. However, the hydraulically significant conductors are constrained to be a subset of the geologic features. The ultimate hydrostructural conceptual model must satisfy both the geology data and the hydraulic information from drilling responses, flow logging, and hydrologic testing. The most efficient result is obtained when the model development is a **continuous integrated interpretation** using all data and not a step-wise processes where geologic and hydraulic data are infrequently and independently reconciled. Hydrochemistry also plays an important role in this integrated interpretation, although such information was incorporated to the model development relatively late in the project.

2.2 Identification of conductive fractures

Already during the TRUE-1 project /Winberg et al, 2000/ the merits of making use of **pressure responses due to drilling** for **hydrostructural interpretation** were identified. In TRUE Block Scale /Andersson et al, 2002a/, with its clearly outlined iterative characterisation methodology, pressure responses to imposed hydraulic disturbances were highly valuable for **identification of conductive** structures in boreholes. In a new borehole being drilled, the position of the drill bit associated with an inflow anomaly (registered in the drilling record) was interpreted as being associated with a hydraulic structure. In the case the flow anomaly was also associated with a simultaneous pressure response in neighbouring boreholes, the observation was taken as an indication of hydraulic connection between boreholes, cf Section 2.3. The hydraulic identification of hydraulic structures was corroborated with geological structures seen in the **borehole TV imaging** (BIPS) and the **core log** (BOREMAP).

Verification and tentative quantification of hydraulic structures identified from flow anomalies were provided by subsequent **flow logging** in the boreholes. Towards the end of the project the Posiva DIFF flow meter /Rouhiainen, 2001/ was utilised exclusively. This tool measures the flow from 1 m sections of the hole using the dilution or travel-time of a heat pulse. The flow resolution is low as 2 ml/min for 76 mm diameter holes. The tool logs the hole in 0.1 m increments, thus providing a resolution of 0.1 m for the location of the flow anomaly. A focused resistivity sensor that is incorporated in the tool further resolves the location of the conductor to within 0.05 m. The joint interpretation based on the flow anomalies and the flow logging were used to identify the *loci* for **focused flow and pressure build-up tests.** These tests were primarily performed on the primary hydraulic conductors found in the boreholes, irrespective of whether they were included in the hydrostructural model at the time, or not. The tests were conducted with a double packer system using the SKB UHT 1 system specially designed for underground hydraulic testing. Towards the end of the TRUE Block Scale Characterisation, a smooth transition was introduced whereby **short-time transient cross-hole interference tests** /e.g. Andersson et al, 2001a,b; Adams et al, 2001/ were conducted in conjunction with tests on selected conductive structures.

The combined interpretation of single hole and cross-hole tests and the BIPS borehole TV data (BOREMAP core log) were used to select the **optimal packer positions** in the borehole within the constraints imposed by the types of multi-packer system employed /Andersson et al, 2002a/.

Geophysical methods, directional borehole radar and various types of cross-hole/3D seismic surveys, were employed during the early stages of the characterisation /Andersson et al, 2002a/. Applications of these methods during the Stripa Project showed some promise that eventually cross-hole geophysics could develop reliable maps of conducting features. The geophysical interpretations of conductive features that were obtained early in the TRUE Block Scale program did not resolve the conductive features of the final hydrostructural model that were determined using geologic and hydraulic data. In the case of the **directional borehole radar** the main problem may be the strong attenuation of the radar signal which is induced by the high salinity of waters in the Äspö HRL. In the case of the **seismic investigations**, the major structures bounding the investigated rock block were possible to identify. However, with the measurement geometry employed (constrained by existing underground openings and available boreholes) could not unambiguously identify the features of the final hydrostructural model.

2.3 Assessment of connectivity and conductive geometry of fracture network

Hydraulic connectivity was essentially assessed in four different ways and for the most part in the following order;

- Pressure responses due to drilling.
- Pressure responses due to hydraulic cross hole interference test.
- Tracer-dilution flow rate responses in one piezometer interval to changes in flow rate from another piezometer interval cf Section 2.2.
- Breakthrough results from tracer tests.

Pressure responses due to drilling were used to identify hydraulic connections. A key component of the iterative characterisation approach is the completion of each borehole with multi-packer piezometers that isolate the significant conducting features. When a new borehole intersects a conducting feature or a conducting network of features, the piezometer intervals that also include that feature or network show clear hydraulic pressure responses. These drilling responses could be compared with predictions based on the hydrostructural model that existed before the borehole was drilled. These comparisons formed a basis for validating or modifying the hydrostructural model /Andersson et al, 2002a/.

Further verification and control of the connectivity of the hydrostructural model, which constituted the basis for the piezometer design, was provided by **long-term cross-hole interference tests**. The results were compiled in so-called **response matrices** to enable easy overview and interpretation. Modelling of pressure responses is discussed further in Section 5.3.

Towards the end of the site characterisation, **tracer dilution tests** constituted a very important ingredient. Tracer dilution tests involve circulating a tracer in a single piezometer interval and monitoring the dilution of that tracer with time. The rate of the dilution is a measure of the groundwater flux through the piezometer interval. The tracer dilution test can be run under either ambient conditions (no pumping anywhere) or pumped conditions (water being injected or removed somewhere). Changes in tracer dilution rates in response to pumping provide clear indications of connection between the observation zone and the pumping zone. These dilution changes occur in a much shorter time than would be required to see breakthrough of a tracer between the two zones. Hence, tracer dilution tests were valuable for indicating which piezometer intervals were likely to provide good breakthroughs for later tracer tests.

On the basis of results obtained predictions could be verified and/or new conductive structures could be added to the list of deterministic structures. An ultimate verification of connectivity was provided by observation of tracer breakthrough in a single structure or an interpreted flow path involving multiple structures, cf Section 3.2.

2.4 Building of hydrostructural models

A hydrostructural model is a three-dimensional map of conductive features that best reconcile the available geologic, hydrogeologic, geophysical, and geochemical data. The hydrostructural model is neither unique (multiple models may be possible) nor is the model free of inconsistencies among different information sources. These uncertainties due to non-uniqueness and inconsistency provide the hypotheses that subsequent characterisation activities are meant to resolve. However, over time and with more data, the hydrostructural model should become more constrained (less non-unique) and resolve a higher portion of available data.

The hydrostructural model consists of the following components;

- Deterministic structures, which have known locations and properties and can be identified in multiple holes from geology and hydraulic data.
- Background conductors, which are defined stochastically based on the geometric and geologic characteristics of conducting features in the boreholes that cannot be assigned to deterministic features.
- Geologic properties of conductors including mineralogy and geochemistry (fracture infillings, fracture coatings, alteration zones around conductors), structural geology (indications of mechanical origin such as slickensides, second-order fracturing), and lithology (preferential fracture characteristics in different rock types).
- Hydraulic properties of conductors (both deterministic and background) including transmissivity, storativity, and diffusivity.

The hydrostructural model is the basis for constructing numerical simulations and for designing further characterisation activities. Each new borehole prompted a review of the hydrostructural model and new versions of the model, which were documented in internal project reports, appeared five times during the project. The initial hydrostructural model was prepared prior to any drilling of the block, and the model rapidly evolved through its first three revisions, which laid out the major conducting features. The last two revisions largely involved confirmation of several major structures that cut across large portions of the block (such as Structures #20, #5, #19 and #10). The later revisions also added or refined additional structures that fill in the network that was targeted for tracer testing (such as Structures #13, #6, #21, #22, #23 and #24).

The **main rock type** in the TRUE Block Scale rock volume is porphyritic quartz-monzonite (denoted Äspö diorite for short) with an age of about 1800 Ma. In addition, smaller portions of a granodioritic/granitic variety called Ävrö granite has been identified as well as **lenses and dikes** of fine-grained aplitic granites. The mineral compositions of the different bedrock types are presented by /Andersson et al, 2002a/. Details on mineralogy and infilling materials associated with conductive structures are provided in Section 3.2.

2.4.1 Geometry and structure

The conductive geometry of the rock block is made up of deterministic NW structures (easy to predict/characterise) and NNW structures (connections more difficult to assess), both sets characterised by **steep dips**. The largest inflows in boreholes are for the most part associated with geologically or geometrically identified conductors belonging to the above sets. Although subhorizontal fractures are abundant, there are **no evidences of deterministic subhorizontal conductive structures**. This finding is also supported by observations from the nearby access and ventilation shafts. Although the integrated 3D seismic evaluation indicates existence of subhorizontal reflectors, these have been interpreted to be of no, or negligible hydraulic significance. However, scrutiny of the hydrogeochemical data provides an indication of a possible subhorizontal structure/lithological body located above TRUE Block Scale rock volume, cf Section 2.5.

The first three boreholes (KA2563A, KI0025F and KI0023B) were required to develop the **basic model of the network of major conductive structures**. The last two boreholes (KI0025F02 and KI0025F03) basically confirmed and refined the initial basic model. The latter included interpretation of four new structures (#21, #21, #23 and #24) and an additional insight into the heterogeneous natures and interrelation of Structures #13 and #21, cf Figures 2-1 and 2-2. The implications of the above finding is that complex numerical models may not be very useful or cost effective until the basic hydrostructural model has matured to a point where the major, controlling features are defined.

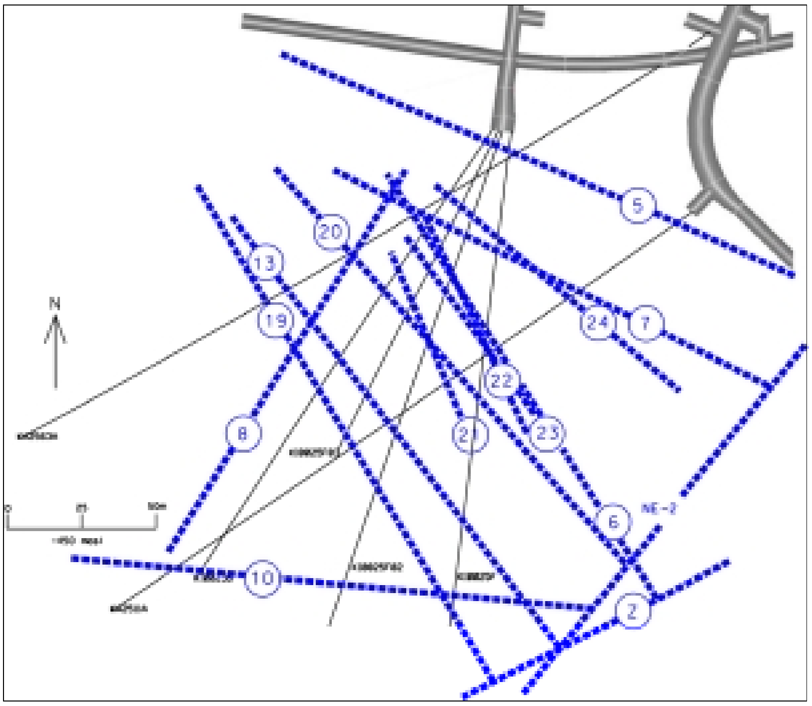


Figure 2-1. Plan view of the Tracer Test Stage hydrostructural model with focus on the target volume of the block /Hermanson and Doe, 2000/.

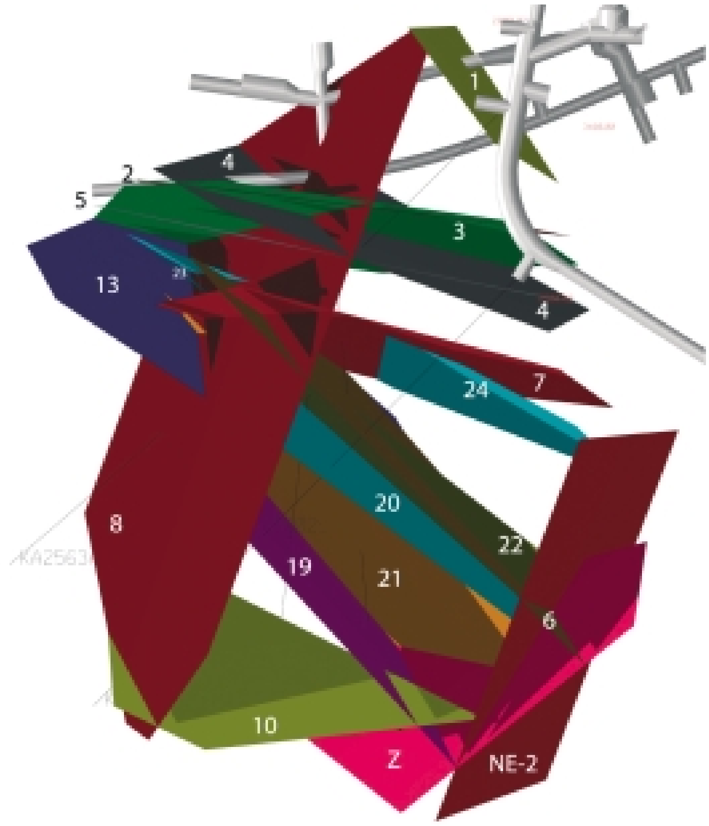


Figure 2-2. *Three-dimensional view of deterministic structural model. View from above including peripheral structures #1–#4, cf Figure 2-1.*

If a hydraulic anomaly supported by an underlying geological/structural and geometric information appears in more than two boreholes, the identified structure was included in the model of **deterministic structures**. The remainder of the conductive fractures/ structures, once the components of the deterministic structural model had been identified, were assigned to a stochastic **background fracture population**. The two sets of background fractures are one NW with steep dips (mean strike/dip 121/89.4) and a less inclined NNW set (mean strike/dip 160/36).

2.4.2 Hydraulic aspects

The **transmissivity of the deterministic structures** which are part of the TRUE Block Scale volume, ranges between $1.5\cdot10^{-9}$ and $3.7\cdot10^{-5}$ m^2/s. The transmissivity of those structures which are involved in the performed tracer tests range between $1.5\cdot10^{-9}$ and $1\cdot10^{-7}$ m^2/s. The **transmissivity distribution of the background fracture population** as derived from flow logs in the tracer test area is found to be log-normal distribution (${}^{10}\log T = -8.95$ and $\sigma_{10\log T}=0.93$). The distributions of transmissivity of the two populations are found to partly overlap. This implies that amongst the background fractures there are conductive structures which, due the geometry of the TRUE Block Scale borehole array, are only known at one interpreted borehole intercept. It should be noted, however, that deterministic structures account for all the major inflows that the flow logs identified. Hence, it is unlikely that there are any major, cross-cutting structures in the block that are not identified as deterministic structures.

Low pressure responses to tests involving Structure #13 have suggested that the structure in question is discontinuous, or possibly that some intercepts interpreted as associated with Structure #13 in fact are associated with a different structure /Hermanson and Doe, 2000/. However, the interpreted discontinuity in Structure #13 is contradicted by associated responses to tracer dilution tests /Andersson et al, 2000a/. An alternative cause for the noted lack of pressure response may be that some other water source acts as a reservoir and constant head boundary that reduces pressure responses to pumping in more distant pumping sections. A possible candidate for such a reservoir is the fracture intersection zone (FIZ) between Structure #13 and #21 that extends close to intersections of Structure #13 in boreholes KI0025F02 and KI0025F03. It should be mentioned that the groundwater chemistry does not indicate a discontinuity in Structure #13. The available data thus supports the interpretation of a continuous Structure #13 as included in the hydrostructural model. The difference in drawdown response is attributed to a flow channel or fracture intersection effect.

Flow geometry has important implications for the movement of tracers in the TRUE Block Scale volume. How many pathways participate in transport and how much surface area do those pathways provide for fracture-rock interaction? Is the flow along pipe-like channels that would produce geometrically linear flow in hydraulic tests? Is the flow confined to two-dimensional planar features, such as the major features of the TRUE Block hydrostructural model? Is there a three-dimensional network of fractures providing the major portion of flow along the pathways of the tracer tests? Flow geometry applicable to the TRUE Block Scale experiments has been investigated by analysing geometric information derived from the pressure data produced during cross-hole hydraulic testing /Doe, 2002/. The results show that all of the monitoring intervals ultimately see constant pressure boundaries or higher dimension flow regions, indicating that all conductive structures have connection to the larger flow systems of the Äspö HRL. For Structure #20 the distance to these boundaries is between 100 m and 250 m, the uncertainty being dictated by the range of diffusivity values (ratios between transmissivity and storativity). It is further noted that the central region of Structure #20 has a lower diffusivity than more distant regions of the structure. This lower diffusivity may indicate a higher porosity region in Structure #20 in the central parts of the experimental area. The region of most interest for performance of tracer tests lies within a portion of Structure #20 that is characterised by Dimension 2 (radial flow) or lower.

2.4.3 Major conclusions

The principal experience from the characterisation and subsequent construction of a hydrostructural model is that it is not possible to decouple structural-geological and hydraulic data/elements in building the hydrostructural model. For the most part the hydraulic information and geological structural information is integrated simultaneously in the interpretation. However, at times a hydraulic anomaly does not have a straightforward corresponding geological/geometrical interpretation, and a more thorough examination of the geological data is required. An example is the identification of Structures #21 and #22 in TRUE Block Scale /Hermanson and Doe, 2000/.

The main set of tools for determining the conductive geometry is a combination of borehole television (BIPS) and flow logging (Posiva difference flow log) and pressure responses (drilling/cross-hole tests).

The major conducting structures and their likely terminations between boreholes have been determined. The basic hydrostructural model was established using information from the three first boreholes. No major changes to the model were required on the basis of the additional information acquired from the last two boreholes. However, additional detail (new structures and insight into heterogeneity) was added to the model.

Difficulties remain with regards to the actual extent of interpreted deterministic structures outside the borehole array. Because the boreholes are sub-horizontal, the block is undersampled vertically, however, we have some interesting insights on the vertical extents of conductors from pressure responses in borehole KA2511A. KA2511A lies above the rest of the borehole array by more than 80 meters in the plane of Structure #20, cf Figure 2-1. Except for Structure #5, at the extreme northeast of the block, and Structure #10, at the extreme southwest of the block, none of the deterministic structures in the TRUE Block Scale rock volume (and none of those used for tracer testing) appear in this hole. The absence of most structures in KA2511A provides a limit on the upward vertical extents of these features.

In terms of hydraulic connectivity and hydraulic response characteristics the interpreted structures form **two main groupings**; the “#20/#13-system” (including #21, #22) and the “#6/#7/#5-system” (including #24), the two of which are featured by distinct differences in response times and response characteristics /Andersson et al, 2002a/. Structure #19 is a major structure cutting through the investigated rock volume that is distinct from the #20/#13 system, but still connected with it. Structure #10 is the deepest positioned conductor relative to the collar positions, and does not appear to have connections with the rest of the block. The relative isolation of Structures #10 and #19 and their behaviour as single features precluded them from being targets for the tracer experiments described in this report, which required a network of structures. The developed hydrostructural model combined with the understanding of the hydraulic behaviour obtained from cross-hole and tracer dilution tests made it possible to identify a target area for well-controlled tracer experiments. The length scales over which tracer tests have been performed are characterised by radial flow as inferred from the analysis of flow geometry.

2.5 Conceptual flow model

The overall controls of a groundwater flow system are geometry, material properties and boundary conditions. The boundary conditions in combination with the geometry and material properties will decide the distribution of groundwater head. The distribution of groundwater head in combination with material properties governs the distribution of groundwater flow. The ambient groundwater flow distribution in turn will govern the exchange of naturally occurring solutes in the studied rock block. The basic geometrical control of the groundwater flow system at the TRUE Block Scale site is provided by the hydrostructural model described in Section 2.4. As discussed above, the hydrostructural model completely accounts for the major flow anomalies and cross-hole interferences among the boreholes. Each of the major conductors has been associated with an interpreted intercept of a deterministic structure with an associated structural and mineralogical/geologic description.

Material properties, both in terms of point-wise single hole transmissivity data from flow logging and single flow and pressure build up tests and transmissivities obtained from cross-hole interference tests are available. These results assign material properties to the deterministic structures of the hydrostructural model. Superimposed on the geometric control exerted by the hydrostructural model are the **boundary conditions** imposed by the underground openings (including the cylinder-shaped access tunnel and the shafts) which provides the ultimate hydraulic sink, and provides a general hydraulic gradient in the TRUE Block Scale rock volume directed NNE, cf Figure 2-3. All test sections in the TRUE Block Scale borehole array are connected to the Äspö HRL Hydro Monitoring System (HMS). Given that the borehole array has been under development from 1996 to 1999, it is possible to link responses in the investigated block to global man-made disturbances or natural annual variations.

Due to drainage into the underground openings, the hydraulic head has fallen by as much as 5 m in some intervals over the period of monitoring. However the pattern of the head contours and the gradients in the middle of the block have not changed significantly. The **hydraulic gradient** in the central part of the TRUE Block Scale rock volume was about 0.05 m/m with an observed steeper gradient close to the underground openings. Head data were also found to be essentially consistent within each structure, which provides support for the structural interpretation made /Andersson et al, 2002a/. The number of head data and their distribution, as given by the piezometer array, are in this context deemed to be sufficiently good to allow **assessment of flow directions**, correlation to structures of the hydrostructural model etc. Specifically there is a clear separation in hydraulic head between the various structures going from the interior (Structure #10) to the structure closest to the tunnel (Structure #5) /Andersson et al, 2000a/. In addition, point measurement of **ambient background groundwater flow** has been performed using tracer dilution tests at 22 points distributed over the borehole array. Flow rates generally vary between a few ml/hr up to about 1000 ml/h.

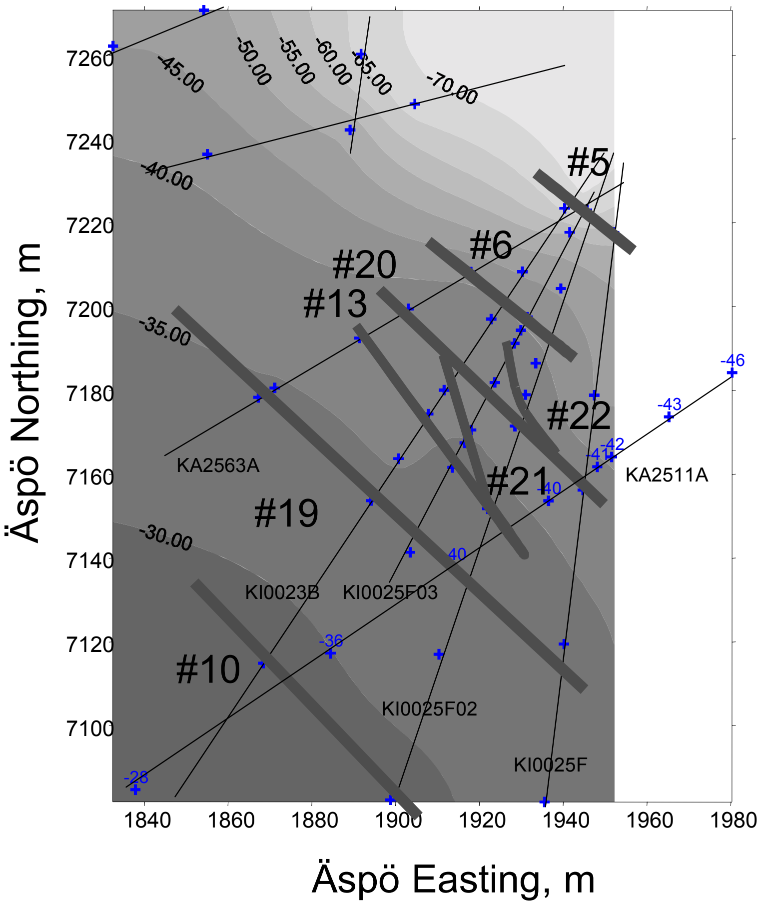
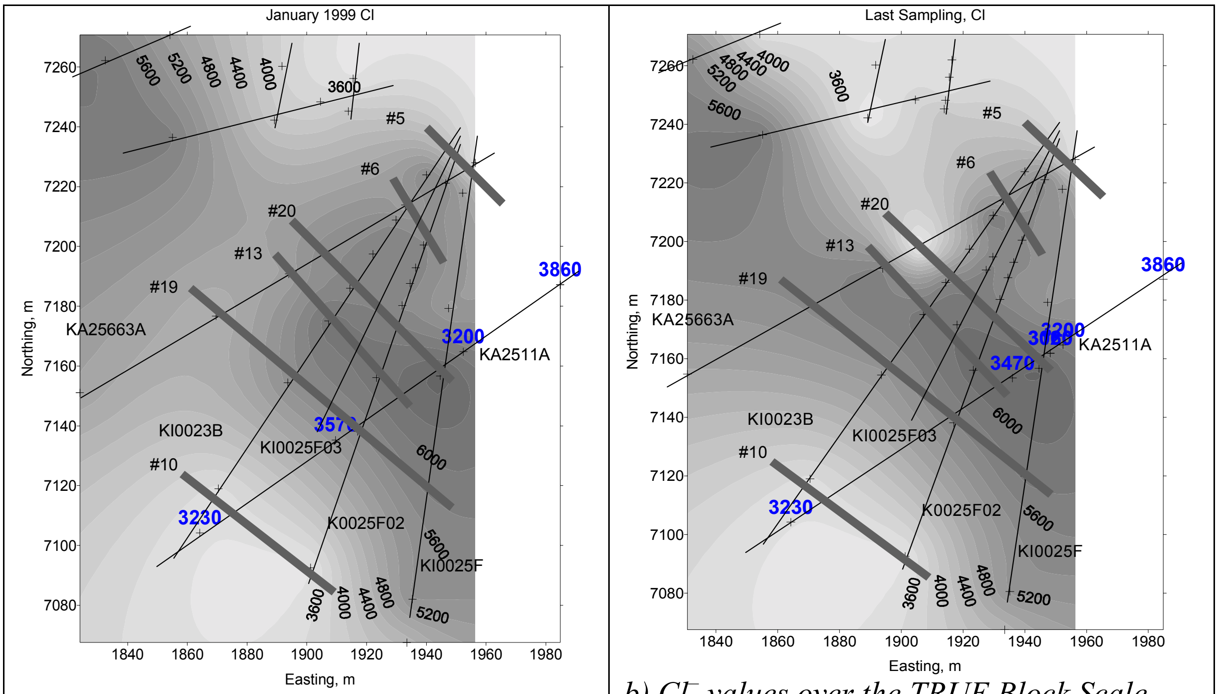


Figure 2-3. Interpolation of measured hydraulic head (masl). Datum is elevation z=0 (mean sea level).

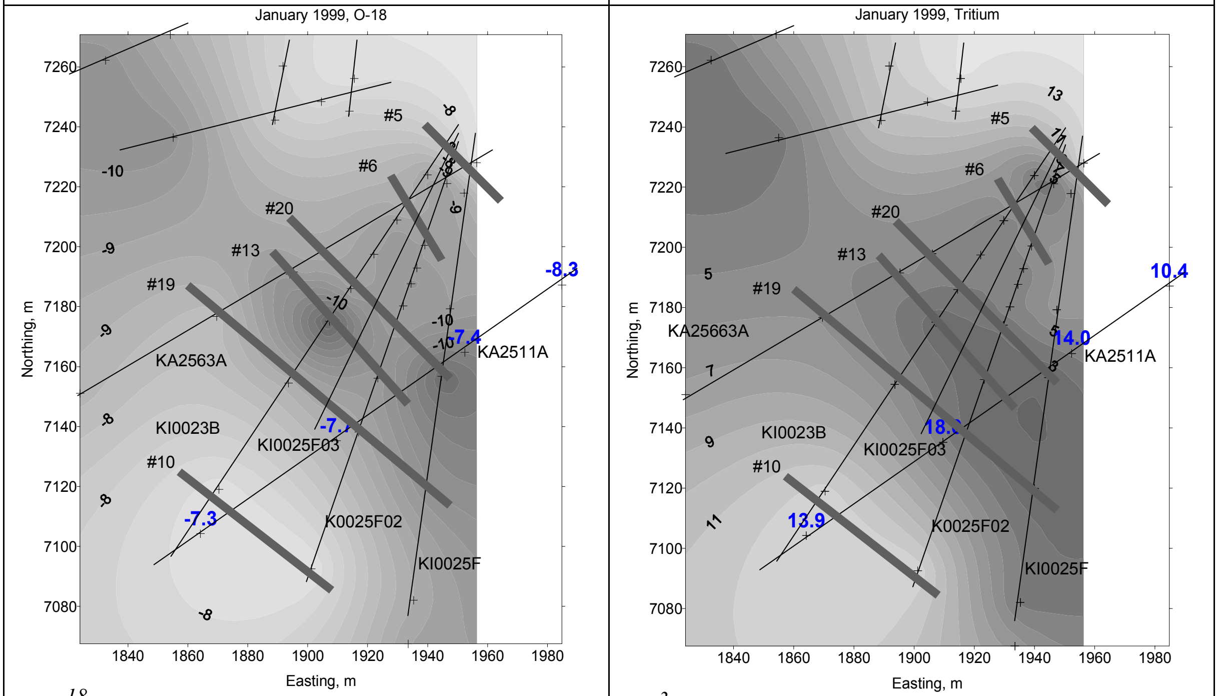
The **flow of water to the underground openings** has affected the **time and space distribution of groundwater chemistry**. Mapping of these changes provide information (and support) on flow patterns and connectivity of the fracture networks in the studied rock volume to larger structures at the Äspö HRL. The information of these variations comes from fluid resistivity logging of open boreholes and from chemical analyses of water samples collected in packed-off sections in the piezometers of the borehole array.

The **origin of groundwater** sampled in the TRUE Block Scale array has been mapped primarily using Cl^{-}, $\delta^{18}O$ and ^{3}H. Salinity measured by Cl^{-} is not sufficient to differentiate the two possible sources – Deep brine and Baltic Seawater. The two likely sources differ, however, in their $\delta^{18}O$ values and their exposure to recent bomb-pulse radioisotopes (^{3}H). Groundwater with a large component of Deep brine should have lower ^{3}H and $\delta^{18}O$ than saline waters of Baltic seawater origin /Andersson et al, 2002a/.



a) Cl⁻ values over the TRUE Block Scale rock volume, January 1999.

b) Cl⁻ values over the TRUE Block Scale rock volume last sample values showing low chloride waters entering Structure #20 in KA2563A.



c) $\delta^{18}O$ over the TRUE Block Scale rock volume, January 1999.

d) ^{3}H values over the TRUE Block Scale Volume, January 1999.

Figure 2-4. *TRUE Block Scale Rock volume. Interpolated chemical variables /Andersson et al, 2002a/.*

Figure 2-4 shows the Cl^-, $\delta^{18}O$ and ^3H plots for water collected in January 1999. The plot clearly shows that different water types occupy different parts of the network of structures in the TRUE Block Scale rock volume. For example, Baltic seawater (low Cl^-, high $\delta^{18}O$ and high ^3H) is evident in the area of Structure #10 and the lower parts of boreholes KI0023B, KI0025F02 and KA2511A. Water that seems to be a mix of Deep brine and Glacial water is associated with Structures #20 and #13. Comparing Figure 2-4a and 2-4d (the latter showing last results) a gradual invasion of much fresher water in the area of the Structure #20 intercept in borehole KA2563A is evident. The source of this water is believed to be the same providing the source for water collected in borehole KA2511A, see below.

Similarly, the water collected in boreholes KA2511A (borehole located up to several tens of meters above the centre of the borehole array) are dominated by more fresh, Baltic seawater dominated water. The observed differences in hydraulic head as well as the chemical information indicated a hydraulic discontinuity between the centre of the TRUE Block Scale rock volume and the overlying borehole KA2511A. The piezometer sections of KA2511A are well connected over the length of the hole. This connection has been extensively studied to eliminate the possibility of equipment malfunctions. The connectivity of the KA2511 piezometer sections suggests the existence of subhorizontal discontinuity that has not yet been penetrated by a borehole.

2.6 Borehole array – its potential and limitations

The TRUE Block Scale **borehole array** has been developed using collar positions at the 340 m level (KA2511A, KA2563A) and at the 450 m level (remainder of boreholes), cf Figure 2-5. Two of the boreholes are 56 mm cored boreholes (KA2511A and KA2563A) and the remainder is 76 mm cored holes.

Constraints are introduced by the fact that boreholes can only be positioned at pre-existing and accessible niche locations. The location and geometry of the niches from where the boreholes have been sunk restrict the ability to sample NE trending fractures. Given that the main conductive set is NW or NNW, this constraint constitutes a minor problem.

Two independent groups have developed the piezometer **systems** used in the TRUE Block Scale project. The SKB-GEOSIGMA system, which was used for the first boreholes (KA2511A, KA2563A, KI0025F and KI0025F03), use flow and pressure lines that are external to the packer emplacement pipes. The ANDRA-Solexperts system, which was used on subsequent holes (KI0023B and KI0025F02) use a large-diameter pipe for packer emplacement and the flow and pressure measurement lines run internally in this pipe. The SKB-GEOSIGMA system has a capacity of seven piezometer sections with flow circulation (or 21 sections of pressure monitoring only), and the ANDRA-Solexperts system can accommodate ten sections with both circulating flow and pressure monitoring /Andersson et al, 2002a/.

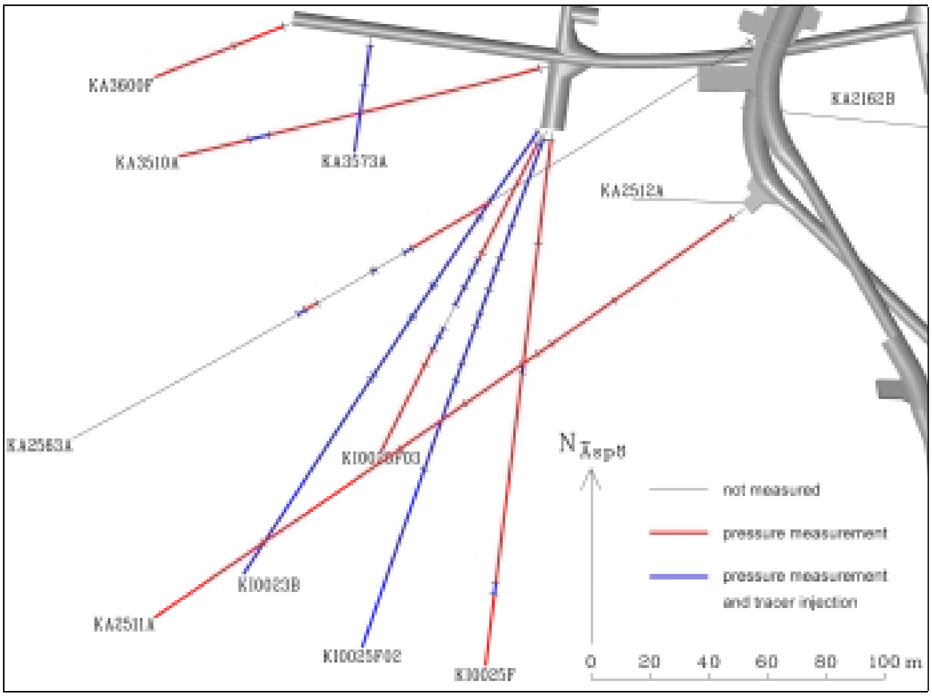


Figure 2-5. *TRUE Block Scale borehole array and definition of defined rock volumes in the investigated rock block. The figure also indicates the locations of packed off intervals in the boreholes (per June 2000).*

The installation in KI0023B suffered a collapse of the central tubing at about 100 m depth. An attempt was made to exchange the faulty components in the borehole, but the piezometer could not be removed from the hole without a risk of losing the hole to stuck equipment. It was however possible to reposition the piezometer at its original location. The inability to repair the piezometer reduced its function in not allowing a flow log with the Posiva system, which was introduced after KI0023B, and the piezometer could not be reconfigured in response to subsequent modifications to the hydrostructural model. In its frozen configuration, the piezometer short circuits Structures #20 and #6 in the same piezometer interval. Fortunately the major flowing feature of KI0023B is not Structure #20, but is Structure #21, which lies within a few metres of Structure #20 at this borehole location. The main remedy to this situation was to use Structure #21 in KI0023B as the main sink for most tracers. Using this interval as a sink reversed the gradient from Structure #6 to Structure #20 in KI0023B thus minimising the impact of the short circuit. The existence of the short circuit did not compromise the objectives of the TRUE Block Scale project, as there was a good selection of pathways through different structures to the targeted sink, the short circuit did constrain the selection of alternative tracer sinks.

The preferred direction of drilling is not considered a serious constraint given that the preferentially sampled fracture set constitutes the principal conductive fracture set at Äspö HRL. Although the goal at all times was to include only a single deterministic structures in each packed off section, some intervals contain multiple structures when the hole intersects the structures near a fracture intersection. The only other potential short circuit exists in borehole KA2563A, where Structures #6, #7 and #21 lie in the same interval. Overall, in light of the performed tracer tests this restriction did not constitute any serious constraint.

During the course of the TRUE Block Scale Project, five hydrostructural model updates where made. These updates were made following completion and characterisation of the new boreholes. The first three holes (KA2563A, KI0025F and KI0023B) identified the major block-cutting structures of the block, Structures #5, #6, #7, #20, #19. The non-connection of most structures to KA2511A complicated the initial efforts. The additional two boreholes (KI0025F02 and KI0025F03) confirmed the existence of the major structures, added some detail on other structures (#13 and #10) and identified additional structures that completed the network for the tracer tests (Structures #21, #22 and #23). The final hole also identified a shallow Structure #24 that is not part of the main network for tracer testing. It is noted that the finding that three boreholes sufficed to provide the necessary description basic description of the TRUE Block Scale rock volume in no way should be regarded as universal.

2.7 Applications to site characterisation and repository development

General recommendations for site characterisation

The experience of the TRUE Block Scale project defines a model **methodology for site characterisation** of fractured rock in the block scale. This model draws as well on experience from other research facilities, mainly Stripa (Sweden), Grimsel (Switzerland) and Kamaishi (Japan). Together these projects provide a basis for proceeding with future block scale characterisation efforts with confidence.

The **recommended tool kit for block scale characterisation**, as defined in the subsequent sections is equally applicable for assessment of block scale rock volumes using **surface boreholes** and investigations in an **underground rock characterisation facility** (RCF). In addition, during the **development of an underground repository** such a methodology can be applied to define **location of storage tunnels and canister positions**.

Although the experience from TRUE Block Scale is drawn from characterisation performed over a limited length scale (< 200 m), the methodology is also largely applicable to investigations on larger scales, e.g. site scale (hundreds of metres to kilometres). However, restrictions in applicability may imposed by a) the length scale itself (i.e. foreseen distances between boreholes) and b) investigations in surface boreholes (smaller hydraulic disturbances possible compared to what can be achieved in an underground situation). An even more important constraint is time. During a site characterisation for a nuclear repository it may be difficult to fully honour a truly sequential and iterative investigation campaign as the one applied in TRUE Block Scale.

Iterative approach to site characterisation and toolbox

One of the principal lessons of the TRUE Block Scale Project is that important and **early information on the geometry of conductive structures/fractures** can be obtained from the drilling process itself. The combined observation of flow anomalies in the borehole drilled paired with pressure responses in an existing piezometer array can provide information on location of hydraulic structures and their connectivity within a given rock block. In order to draw **maximum information from the drilling process**, it should be iterative, by which correlation between flow anomalies and pressure responses is relatively straightforward. In an underground laboratory situation with many projects/activities going on simultaneously such correlation studies call for a system for **accounting of all underground activities and events** such that irrelevant anomalies may be screened out. For a surface drilling campaign, and under practical and logistical constraints, it may be necessary to allow drilling at a given site at multiple locations. If distances between borehole collar positions are sufficient and the relative positions of boreholes are steered by any preconception of compartmentalisation (bounding fracture zones), the information obtained from drilling may still be important and may help planning the successive characterisation steps.

The maximum value of the information obtained during characterisation is realised from a continuous and simultaneous integration of as much information from as many different sources as possible. In the case of TRUE Block Scale the geological/structural information (BIPS, corelog) has been interpreted jointly with hydraulic information (e.g. flow anomalies and pressure responses). During the course of the TRUE Block Scale project a number of different techniques for identifying conductive structures have been investigated/tested. The drilling and the core log provide initial identification. Flow logging provides subsequent verification and tentative quantification of flowing features. The Posiva DIFF flow meter has been found to provide the necessary detail which allows identification of the major conductive structures (absolute flow estimate may be difficult) and at the same time allows identification of minute inflows down to q=2 ml/min which helps define statistics for description of the background fracturing, e.g. the **frequency of conductive fractures**. The majority of the identified flow anomalies can be related to the underlying geological and structural context through the BIPS borehole TV data and the drill core/core log itself.

It should also be noted that careful core drilling using triple-tube technique combined with careful core handling and core logging provide the means for recovery of unconsolidated infillings of fault rock zones (including fault gouge).

In summary, drilling data (flow anomalies), BIPS borehole TV imaging and high-resolution flow logging provides identification of conductive structures over the full range of size and flow rates. Information on connectivity of structures is provided by pressure responses to drilling in existing piezometers. Refinement of such early inferences is provided by subsequent cross-hole pressure interference tests. Flow logging locates conductive fractures and provides an initial estimate of their hydraulic properties. Transient transmissivity data are obtained from a combination of single-hole pressure build up tests and cross-hole interference tests. Hydrochemical information, tracer dilution tests and cross-hole tracer tests provide verification and control of the hydrostructural model.

3 Major accomplishments from laboratory investigations

Three major accomplishments are associated with the laboratory programme associated with the TRUE Block Scale programme /Andersson et al, 2002a/. First, **comprehensive mineralogical and geochemical investigation** of conductor materials, particularly fine-grained gouge provides a strong basis for predicting retention behaviour. The geochemical programme /Andersson et al, 2002a/ included **stable isotopes** (^{18}O and ^{13}C) and **uranium series** analyses on selected samples to provide increased understanding of relative age of fractures and hydrothermal events occurring in them and redox conditions as inferred from relative stability of different uranium isotopes, respectively. The second major accomplishment involves establishment of porosity **distributions** in matrix rock and around altered fractures, which was expanded beyond the TRUE-1 efforts /Winberg et al, 2000/ to include the porosity of mm- and cm-sized **fault breccia fragments and pieces**, respectively. Third, in K_d values were estimated making use of the comprehensive mineralogical and groundwater chemistry database in the absence of direct laboratory-derived sorption data for materials from the conducting structures.

In the following details on the laboratory results are provided with a special emphasis on conductive structures.

3.1 Mineralogy and geochemistry

The lithology of the various bedrock types found in the TRUE Block Scale rock volume is briefly described in Section 2.4.1.

Conductive structures at Äspö are associated with tectonised **rock** in the form of **cataclasites** (recrystallisation of quartz, increased frequency of micro fractures, **variable degree of chemical alteration**) and **mylonites** (complete grain size reduction, recrystallisation/alteration of wall rock) /Andersson et al, 2002a/. The cores and borehole imagery of the structures show alteration and tectonisation of the wall rock. Generally, the widths of the associated cataclastic zone are on the order of centimetres to decimetres whereas the mylonites are from millimetres to a few centimetres wide. Most structures appear to be the result of brittle reactivation of old ductile/semi-ductile deformation zones.

The movements along fault planes have resulted in **fault breccia** and **fault gouge** distributed in variable amounts and proportions over the fracture and structure planes. The fault gouge material is characterised in terms of **grain size distribution** and **mineral composition**. No measurement of its *in situ* porosity exists. Despite that the exclusive use of **triple tube drilling** in the TRUE Block Scale Project, some of the unconsolidated material was inevitably lost during the drilling process. In addition, the samples from the 52 mm size core from the 76 mm hole were not large enough to properly assess the size distribution. However, size analyses of larger samples collected from the tunnel indicate a **power law distribution** with approximate fractal dimensions of 2.1 for an equivalent three-dimensional fracture network. The fault breccia material consists mainly of altered wall rock samples, which may include mylonite fragments. The smaller fractions contain single grains of quartz, feldspars, epidote, chlorite, illite with or without other clay minerals. The very fine fraction (< 0.125 mm) of fault gouge material from Structures #6, #19, #20 and #22 were analysed for main and trace elements, and mineral composition using X-ray diffraction. The **clay fractions** (< 0.002 mm) were analysed separately. Compared to the materials retrieved from fractures in the Redox Zone experiments /Banwart, 1995/ the material from Structures #19, #20 and #22 show larger amounts of clay minerals. Structure #22 in particular shows large amounts of very fine-grained material, mainly consisting of chlorite and mixed-layer clays. The latter also indicating a anomalously high Cs content (62 ppm), indicative of naturally occurring sorption processes.

3.2 Porosity and porosity distribution

Determination of **connected porosity** in conjunction with the TRUE Block Scale Project was carried out using **water saturation** and **PMMA** (polymethylmethaacrylate) **impregnation** techniques.

The former technique was carried out on unaltered and altered **wall rock samples** from cores, as well as on centimetre sized **fault breccia pieces/fragments**. The resulting proposed representative values are shown in Table 3-1 and in Figure 3-4. The determined porosity values are in close accord with results of previously performed studies /Andersson et al, 2002a/.

Table 3-1. Proposed representative values of connected porosity for geological constituents of a typical structure in the TRUE Block Scale rock volume. Values are based on water saturation porosity data from site-specific material and literature data from /Eliasson, 1993/ and /Mazurek et al, 1997/, cf Figure 3-4.

Geological constituent	**Connected porosity (vol%)**
Fresh Äspö diorite	0.45 +/–0.2
Altered Äspö diorite/cataclasite	0.45–1.5
Mylonite	0.3–0.6
Fault breccia pieces (cm size)	0.3–2.0
Fault breccia fragments (mm sized)	1.5–3.0

An assessment of the distribution and orientation of connected pores was achieved by employing impregnation of samples with ^{14}C-labelled PMMA /Kelokaski et al, 2001/, see also /Andersson et al, 2002a/ for description of method.

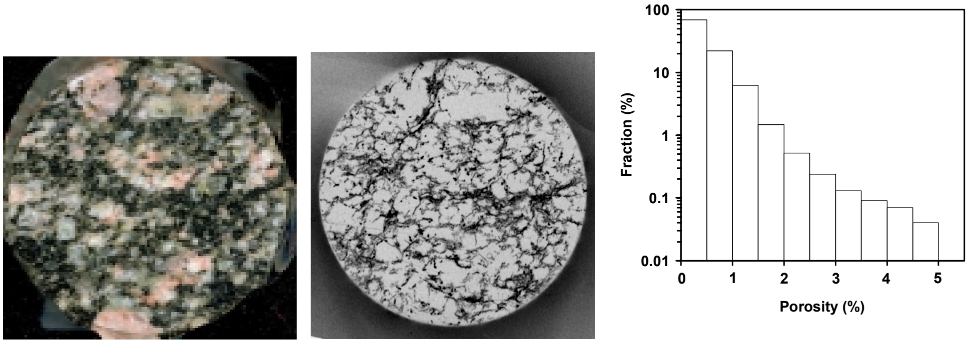


***Figure 3-1.** Results of PMMA impregnation of an intact Äspö diorite sample, a) Photograph, b) Autoradiograph, c) Area fraction with different porosity.*

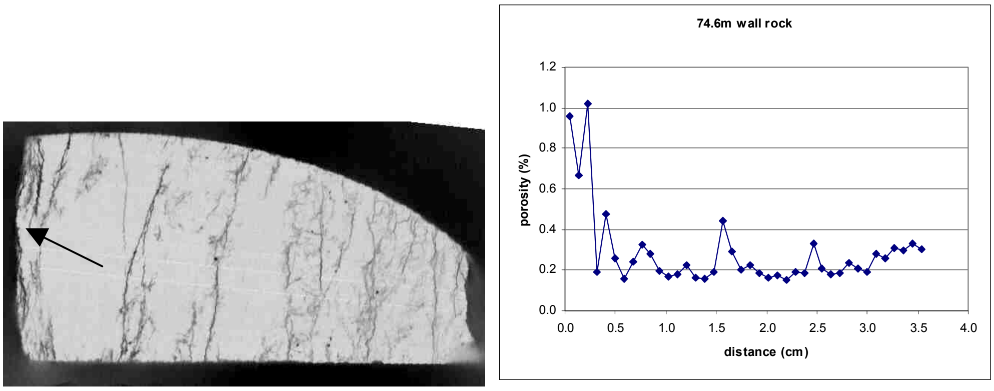


***Figure 3-2.** Results of porosity profiling in wall rock of Structure #20 as obtained from a sample from KI0025F02:L=74.6 m. Arrow indicating fracture surface.*

The heterogeneous nature of the distribution of porosity is shown in Figure 3-1, which depicts an autoradiograph and a porosity distribution determined from a ^{14}C-PMMA impregnated sample. Of the exposed area, 70% of the fracture plane has a porosity less than 0.5 vol-% whereas high porosities (3–5 vol-%) are encountered in < 0.5% of the area. Previous studies, e.g. /Byegård et al, 2001/, have shown evidence of increased porosity in the **altered rim zone** in the vicinity of a conductive fracture. A **decreasing trend normal to the fracture** was also noted. This is also evident in the example from Structure #20 shown in Figure 3-2.

Results of PMMA-impregnation of fault breccia pieces indicate bulk porosities in breccia pieces is similar to that found in the wall rock (0.4–0.8 vol-%) and a porosity of breccia fragments of 1–3%. Breccia pieces from Structure #20 (Figure 3-3) indicate presence of several relatively **extensive micro-fractures**, some of them fully penetrative and forming a connected network. The widths of the micro fractures are in the order of tens of micrometers. Due to the heterogeneous nature of the porosity distribution, the porosity locally exceeds the bulk porosity significantly /Kelokaski et al, 2001/, that is some breccia fragments show porosities > 10%, possibly associated with halos of residual gouge coatings.

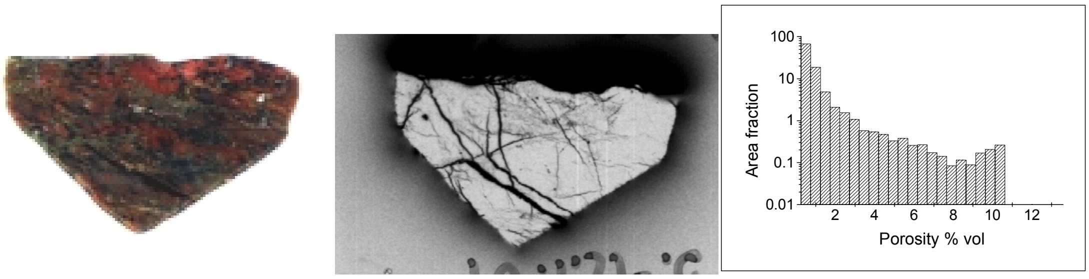


Figure 3-3. *Composite showing a photograph of a cut surface of a cm sized PMMA impregnated fault breccia piece from KI0023B:L=69.9 m (Structure #20) (left), the associated autoradiograph (centre) and the histogram accounting for the area distribution of porosity (right). The total porosity assessed from the exposed surface is 0.8%.*

3.3 Retention properties of geological materials

No laboratory experiments were carried out on site-specific geological materials from TRUE Block Scale. Based on the geological and mineralogical kinship between Feature A investigated in TRUE-1 and the TRUE Block Scale structures, in particular Structure #20, laboratory retention data from TRUE-1 have been used. In the case of fine-grained fault gouge, distribution coefficients have been estimated. The processes and immobile zones involved in TRUE Block Scale as well as the procedure for estimating K_d values for fine-grained fault gouge are described below.

1. Sorption on the fault gouge material in the fractures: Due to the heterogeneity observed for this material, this process has been divided into two types of estimates:
    a. Sorption on the fine-fraction clay-rich fault gouge material: No experimental determination of the sorption parameters of this material is available. An alternative approach has therefore been used where the **sorption coefficients** have been **estimated** using the associated **mineralogical analysis** combined with **cation exchange capacities** (CEC) from the literature and **selectivity coefficients** determined in the TRUE-1 programme /Byegård et al, 1998/ as the basic input.
    b. Sorption on the coarse fraction of the fault breccia material (pieces and fragments): Since no experimental determinations are available for this material, the sorption coefficients determined for the 1–2 mm altered Äspö diorite in the TRUE-1 programme /Byegård et al, 1998/ have been chosen as the best available representative estimates for this material.
2. Surface sorption on the fracture walls. Experimental data are available from the TRUE-1 programme /Byegård et al, 1998/.
3. Diffusion into, and sorption within the rock matrix. Experimental data are available from the TRUE-1 programme /Byegård et al, 1998/.

In the following the procedure employed for item 1a is described briefly.

Table 3-2. Calculated K_d for the different gouge material, size fraction < 125 µm.

Element	Selectivity coefficient K_c	Structure #6 KA2563A:154 m		Structure #19 KI0025F02:133 m		Structure #20 KI0023B:69.9 m		Structure #22 KI0025F02:66.7 m		Crushed material[E] < 63 µm	
		CEC=51 µeq/g (calculated)		CEC=159 µeq/g (calculated)		CEC=54 µeq/g (calculated)		CEC=84 µeq/g (calculated)		CEC=38±6 µeq/g (measured)	
	K_c	Water conc. (M)[A]	K_d (m³/kg)	Water conc. (M)[B]	K_d (m³/kg)	Water conc. (M)[C]	K_d (m³/kg)	Water conc. (M)[D]	K_d (m³/kg)	Water conc. (M)[F]	K_d[G] (m³/kg)
Na^+	0.1[H]	8.3e-2	6.6e-5	8.6e-2	2.0e-4	8.8e-2	6.8e-5	8.8e-2	1.1e-4	9.0e-2	4.7e-5
Mg^{2+}	11[I]	1.7e-3	4.7e-3	1.8e-3	1.4e-2	1.7e-3	4.8e-3	1.9e-3	7.4e-3	1.7e-3	3.3e-3
K^+	66[I]	2.2e-4	1.7e-3	2.0e-4	5.2e-3	2.2e-4	1.8e-3	2.4e-4	2.7e-3	2.1e-4	1.2e-3
Ca^{2+}	1	3.4e-2	4.2e-4	3.5e-2	1.3e-3	3.5e-2	4.4e-4	3.4e-2	6.7e-4	3.7e-2	3.0e-4
Rb^+	2.00E+03[H]	3.3e-7	9.3e-3	3.3e-7	2.8e-2	3.4e-7	9.7e-3	3.6e-7	1.5e-2	3.5e-7	6.7e-3
Sr^{2+}	1[H]	2.1e-4	4.2e-4	2.3e-4	1.3e-3	2.5e-4	4.4e-4	2.7e-4	6.7e-4	2.7e-4	3.0e-4
Cs^+	2.00E+05[H]	1.8e-8	9.3e-2	1.8e-8	2.8e-1	1.8e-8	9.7e-2	1.8e-8	1.5e-1	1.8e-8	6.7e-2
Ba^{2+}	20[H]	4.2e-7	8.5e-3	4.2e-7	2.5e-2	4.3e-7	8.7e-3	4.3e-7	1.3e-2	4.3e-7	5.9e-3

[A] Major components from KI0025F, 164–168 m, [Rb], [Ba] and [Cs] = average of all performed trace element measurements.

[B] Major components from KI0023B, 41.45–42.45 m, [Rb], [Ba] and [Cs] = average of all performed trace element measurements.

[C] Water composition from KI0025F02, 73.3–77.25 m.

[D] Water composition from KI0025F02, 64–72.3 m.

[E] Average of the material used in the investigation by /de la Cruz et al, 2001/.

[F] Average of the water composition of the intercepts for the location of the material used in the investigation by /de la Cruz et al, 2001/.

[G] Uncertainties in the range 10–20% due to the variations observed in the CEC and the water composition.

[H] Value from TRUE-1 investigation of altered Äspö diorite, sampled at KXTT2, 15.1 m /Byegård et al, 1998/.

[I] Value from investigation of Finnsjön granodiorite /Byegård et al, 1995/.

The estimation of the cation exchange capacity (CEC) has been made using the mineralogical composition of the < 0.125 mm material and the CEC of the "pure" minerals found in the literature, cf Section 3.1 and /Andersson et al, 2002a/ and the measured groundwater composition in the relevant test sections. According to the cation exchange model, the part of the cation exchange capacity occupied by a particular cation is determined by the selectivity coefficient for the studied cation relative to a selected reference cation. In the case of TRUE Block Scale, Ca^{2+} was selected as reference since it is found to occupy the major part of the CEC in groundwater-bedrock systems /Andersson et al, 2002a/.

The resulting data for Structures #6, #19, #20 and #22 are shown for reference in Table 3-2. Among the structures involved in the TRUE Block Scale tracer tests, the highest K_d for Cs is noted for Structure #22 (0.15 m^3/kg) . This is attributed to the high content of clay noted for this structure, cf Section 3.1. The overall highest K_d calculated for Cs (0.28 m3/kg) is noted for Structure #19. This value is attributed to its very high overall CEC (159 μeq/g), which is 3 times higher than the corresponding value for Structure #20 (54 μeq/g). For comparison, values of K_d's based on the average of the CEC determined by /de la Cruz et al, 2001/ on crushed wall rock material (< 63μm) are also presented in Table 3-2. The noted difference of the latter values compared to those estimated for the very fine gouge material is attributed to a higher clay mineral content in the fine-grained fault gouge material.

As an additional means of comparison Table 3-3 provides the K_d values attributed to the fault gouge fraction 0.125 to 2 mm. These data are based on investigations on the 1–2 mm fraction of altered Äspö diorite from the TRUE-1 site /Byegård et al, 1998/. It is found that the K_d values for the < 0.125 mm fraction are about 20 to 60 times higher than those attributed to the coarser fraction.

Table 3-3. Estimated K_d for the gouge material, size fraction 0.125–2 mm.

Cation	K_d (m^3/kg)	Remark
Na^+	3e-6	B
Mg^{2+}	3e-4	C
K^+	1e-4	C
Ca^{2+}	3e-5	B
Rb^+	9e-4	A
Sr^{2+}	4e-5	B
Cs^+	1e-2	A
Ba^{2+}	1e-3	A

A Sorption coefficient, measured in batch experiment from the loss of the tracer in the aqueous phase.

B Desorption coefficient, measured in batch experiment from the desorption of the tracer.

C Calculated using the average ratio of the K_d-values found for Mg/Ca and K/Ca, respectively, cf Table 7-4 in /Andersson et al, 2002a/.

3.4 Generalised detailed conceptual model of target structure

The conceptual model for a typical TRUE Block Scale conductive structure (Figure 3-4) is a composite drawn mainly from Structure #20, the primary structure of the core region of the TRUE Block Scale rock volume, with some input from Structures #13 and #22. /Andersson et al, 2002a/. The lower part of the figure highlights the existence of a **altered rim zone** centred on a **mylonitic precursor** with cataclastic insertions. It is noted that it is anticipated that the **number of conductive fractures** may vary along the extent of the structure. Brought to a larger scale /Andersson et al, 2002a/ the number of master faults may also vary considerably along the extent of a structure. One lesson learned from these investigations is not to extrapolate the appearance of a structure in a single borehole intercept as being valid for the full extent (100–300 m) of a deterministic structure.

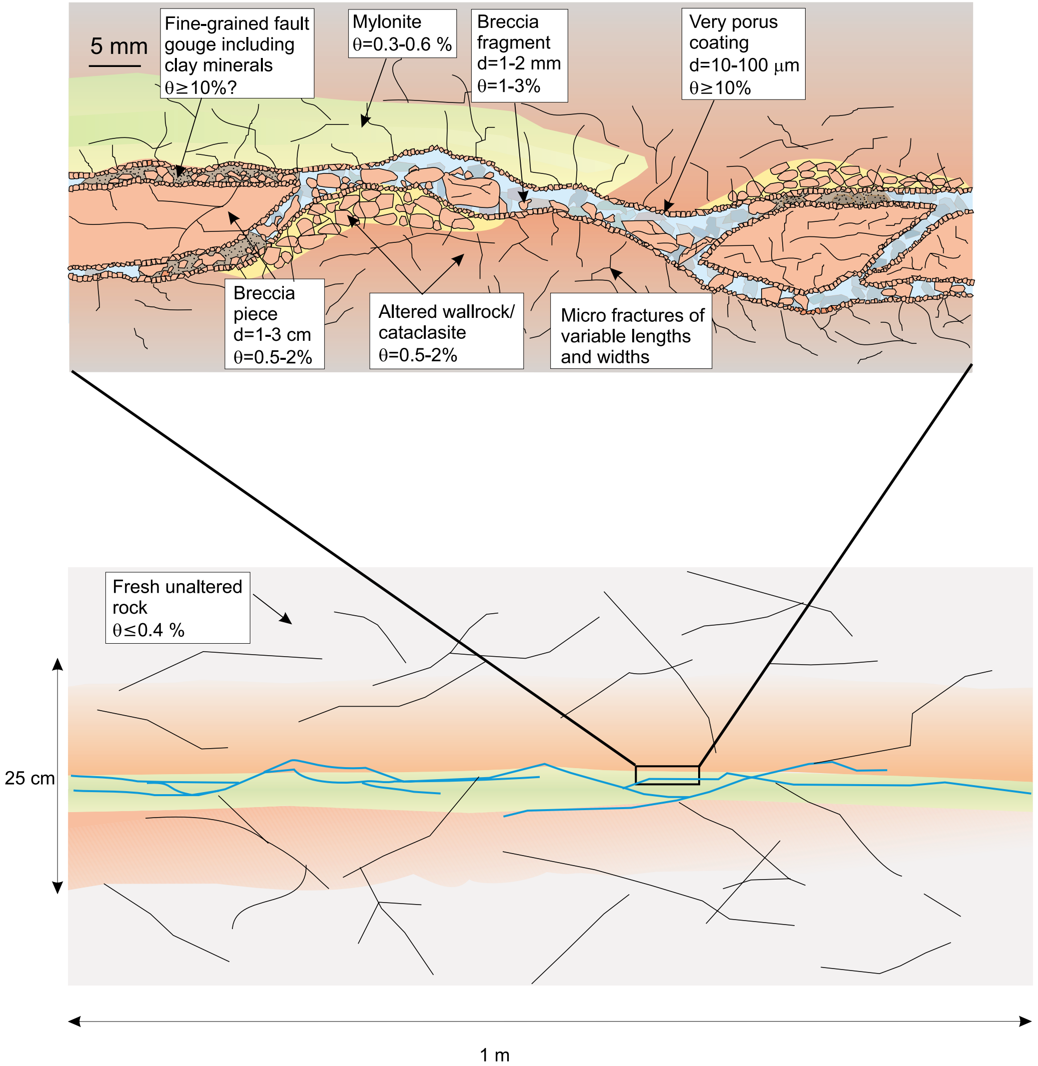


Figure 3-4. Generalised conceptual model of a typical conductive structure involved in the tracer experiments. Details on porosity estimates are provided in Section 3.2.

The upper part of the figure details the typical composition of the altered rim zone. The zone is featured by a thin highly porous layer (10–100 µm) in direct contact with the flowing water in the fractures. The porosity decreases normal to the fractures to attain the average porosity of the unaltered rock ($\theta \leq 0.4\%$) at some distance away from the fracture wall. In accordance with the findings in Section 3.2 it is also assumed that the porosity accessible along the flow paths is heterogeneously distributed. The fracture planes are to a variable degree in-filled with fault breccia (i.e. cm-sized pieces and mm-sized fragments and a matrix of fine-grained clayey fault gouge). It is envisaged that the distribution of in-filling materials is variable such that variably shaped open spaces (physical flow channels) occur. The actual active flow channels that will develop for a given flow situation are dependent on the actual hydraulic boundary conditions.

4 Major accomplishments from block scale tracer tests

During the TRUE Block Scale project different types of tests with tracers have been conducted at various times and with different objectives. Early tests had the objective of showing the **feasibility** of conducting cross-hole tracer experiments in the block scale (L=10–100 m). These tracer tests were carried out in conjunction with cross-hole pressure interference tests. **Tracer dilution tests** were also performed in conjunction with cross-hole interference tests. The latter tests were perhaps the most important of the pre-tests. The dilution tests were used **to identify and screen among possible injection points** and to provide additional information to **verify the current hydrostructural model**. For the selected testing intervals, these tests were conducted both under ambient flow conditions and pumping conditions. A large pressure response (drawdown) combined with an increased rate of tracer dilution were favourable criteria for selecting tracer test injection points.

In addition to the tracer dilution tests, a large number of **cross-hole tracer tests** were subsequently performed with the ultimate objective to select the tracer test geometry (source-sink combinations) suitable for tests with radioactive sorbing tracers. The main factor for this selection was the **tracer mass recovery**. Even though the main purpose of cross-hole tests was to verify connectivity and mass recovery and help to select flow paths for retention experiments, a secondary objective was to actually **characterise the flow paths**, i.e. to determine advective transport properties. A secondary objective coupled to transport was also to study possible effects of fracture intersection zones (FIZ). The experimental programme was crowned by the series of four injections of radioactive sorbing tracers over length scales of 15–100 m as inferred from the hydrostructural model.

The **key design challenge** with tracer tests run on **larger length scales** was to select a test geometry, which produced both sufficiently **high mass recovery**, and analysable breakthrough curves for cross-hole sorbing tracer tests **within reasonable time frames**. Experience from the TRUE-1 experiments /Winberg et al, 2000/ showed that tracer dilution tests in combination with cross-hole interference produced data that could predict the success of potential injection and pumping points for tracer tests.

4.1 Experimental programme

Strategies

Within the TRUE Block Scale Experiment a series of tracer experiments have been performed with varied objectives and scope. Early on in the project the ambition was directed towards demonstrating that block scale tracer tests, over distances > 10 m, where feasible and provided reasonable results. Such demonstration was provided already by late 1998 /Andersson et al, 2001a; Winberg, 1999/. Subsequently, tracer breakthrough (although not with high mass recovery) was demonstrated for a wide range of distances /Andersson et al, 2001b; Winberg, 2000/. Subsequent efforts leading up to performance of a series of four injections with radioactive sorbing tracers were preceded by evaluation of **alternative sink sections** (Phase A) /Andersson et al, 2000a/ **and demonstration of satisfactorily high mass recovery** (> 80%) for source sections to qualify as injection sections for radioactive sorbing tracers (Phase B) /Andersson et al, 2000b/.

The iterative strategy successfully led to the Phase C tests /Andersson et al, 2001c/ with **radioactive sorbing tracers** over Euclidean distances varying between 16–33 m (14–97 m interpreted along the developed hydrostructural model). It is noted that the successive evaluation of the Phase C tests /Andersson et al, 2002b; Poteri et al, 2002/ have indicated that the previously projected flow paths for the C2 injection were shorter than the projected 97 m. Likewise, the interpreted single structure flow path along Structure #21 tested by the C3 injection turned out to be much more complicated than originally thought.

Techniques and methodology

The critical component when exploring alternative block scale tracer test set-ups is the **identification and ranking of potential source sections**. Within the TRUE Block Scale Project a combination of observed pressure responses associated with a given sink and the corresponding flow anomalies from tracer dilution tests provided a strong basis for identifying viable source-sink combinations.

The basic elements of the tracer test methodology were imported from the detailed scale tracer tests performed within the scope of the First TRUE Stage (TRUE-1), /Winberg et al, 2000/. New elements in the methodology were 1) the types (forms) of tracer input signals employed and 2) on-line monitoring on both the injection and pumping sides, /Andersson et al, 2002b/. With regards to the former point, experiments in TRUE Block Scale were performed using **decaying pulses** and **finite pulses** (using exchange of water in the circulation loop) introduced in **radially converging flow geometries**. These procedures built on experiences from the TRUE-1 tests /Winberg et al, 2000/. However, for some potential source sections, the flow rate was considered too small to produce acceptable mass recovery in the context of radioactive sorbing tracers. For these source sections an **imposed injection flow rate** (over-pressure) was applied, resulting in a strongly **unequal dipole** (~ 1:50).

Tracers used

In performing the tracer tests, both conservative tracers (fluorescent dyes, metal complexes and radioactive) and radioactive sorbing tracers were employed, and often administered in cocktails including many different tracers. In the selection of the tracers, experience from the TRUE-1 experiments /Winberg et al, 2000/ were taken into consideration. **Sorbing (reactive) tracers** were selected among the elements of the **alkali and alkaline earth metal groups** previously used in the TRUE-1 experiments /Winberg et al, 2000/. These are characterised by **ion exchange** as the main sorption mechanism. General observations from the TRUE-1 *in situ* experiments were the following; Na^+, Ca^{2+} and Sr^{2+} were transported only very slightly retarded compared with the non-sorbing tracers, Rb^+ and Ba^{2+} moderately retarded and Cs^+ strongly retarded. Using the concept of a retardation coefficient for each tracer, it was identified as necessary to use tracers like Rb^+, Ba^{2+} and Cs^+ to be able to observe a significant retardation. However, it was also considered likely that transport over longer distances (like in TRUE Block Scale) would result in increased retardation, and that breakthrough would only be obtained from slightly/weakly sorbing tracers (like Na^+, Ca^{2+} and Sr^{2+}). It was therefore decided that at least one slightly sorbing tracer and one strongly sorbing tracer should be used in each injection.

Apart from the radioactive sorbing tracers, **radioactive non-sorbing tracers** were used as a complimentary conservative reference, e.g. $^{82}Br^-$ in injection C1, $^{186}ReO_4^-$ in injection C2, HTO (tritiated water) in injection C3 and a combination of $^{82}Br^-$ and $^{131}I^-$ used in injection C4. The radioactive non-sorbing tracers used in the injections C1 and C2 were rather short-lived and it was therefore decided to also use Uranine (C1) and Naphtionate (C2) as complementary conservative tracers. The C4 injection, conducted in the source-sink set-up previously used for the C1 injection (NB C4 was not part of the dedicated Phase C prediction/evaluation process), employed sorbing tracers with an **alternative sorption mechanism** featured by partial hydrolysis of cations and surface complexation (^{54}Mn, ^{57}Co and ^{65}Zn). The objective with the latter tests was to verify results from the laboratory of a retardation of the tracers used being in accord with their hydrolysis constants /Andersson et al, 2001c/.

4.2 What has been learned about the studied flow paths

The TRUE Block Scale tracer test programme involved 14 tracer test campaigns, performance of 32 conservative tracer injections in 16 different combinations of source and sink pairs (flow paths) as shown in Figures 4-1 and 4-2. Of the 16 flow paths tested, three did not produce any measurable breakthrough. The TRUE Block Scale *in situ* tracer test data set is one of the largest ever collected concerning transport of solutes in fracture networks in fractured crystalline bedrock over distances ranging from 10 to 130 m. Of the tested flow paths 8 constitute **single structure flow paths** (six in Structure #20 and two in Structure #21), whereas the remaining 8 paths constitute flow paths which are interpreted to involve multiple structures (**network flow paths**) on the basis of the final hydrostructural model, cf Table 4-1. In the following, a discussion follows of single structure flow paths and network flow paths. In subsequent sections, the flow paths in which tests with radioactive sorbing tracers have been performed are discussed on an individual basis.

Table 4-1. Summary of flow paths tested by tracer tests in the TRUE Block Scale Project.

Flow path no	Source	Sink	Structures	Distance (m)*	Tests	Comment
I	KI0025F03:P5	KI0023B:P6	#20,21	14 (16)	A-4, B-1, B-2, C1, C4	
II	KI0025F03:P7	KI0023B:P6	#23,21	17 (97)	A-4, B-2, C2	
III	KI0025F02:P3	KI0023B:P6	#13,21,#22	33 (33)	PT-4, B-2, C3	
IV	KI0025F03:P6	KI0023B:P6	#22,21	15 (73)	A-4, B-1, B-2	
V	KI0025F03:P3	KI0023B:P6	#21	27 (27)	B-2	
VI	KI0025F02:P5	KI0023B:P6	#20,21	21 (21)	B-1	
VII	KI0025F02:P6	KI0023B:P6	#22,21	18 (65)	PT-4, B-2	
VIII	KA2563A:S1	KI0023B:P6	#19,21	55 (130)	PT-4, B-2	
IX	KA2563A:S4	KI0023B:P6	#20,21	16 (16)	ESV-1c, PT-4	
X	KI0023B:P4	KI0023B:P6	#13,21	15 (48)	ESV-1c	No bt at 220 h
XI	KI0025F:R4	KI0023B:P6	#20,21	42 (47)	ESV-1c	No bt at 220 h
XII	KI0025F02:P3	KI0025F03:P5	#13,21,20	26 (37)	A-5	No bt at 643 h
XIII	KI0025F02:P5	KI0025F03:P5	#20	11 (11)	A-5	
XIV	KI0025F02:P6	KI0025F03:P5	#22,20	12 (57)	A-5	
XV	KI0025F03:P6	KI0025F03:P5	#22,20	12 (65)	A-5	
XVI	KA2563A:S4	KI0025F03:P5	#20	29 (29)	A-5	

* Distance in space (Euclidean), distance within brackets = distance along interpreted deterministic structures.
bt = breakthrough.

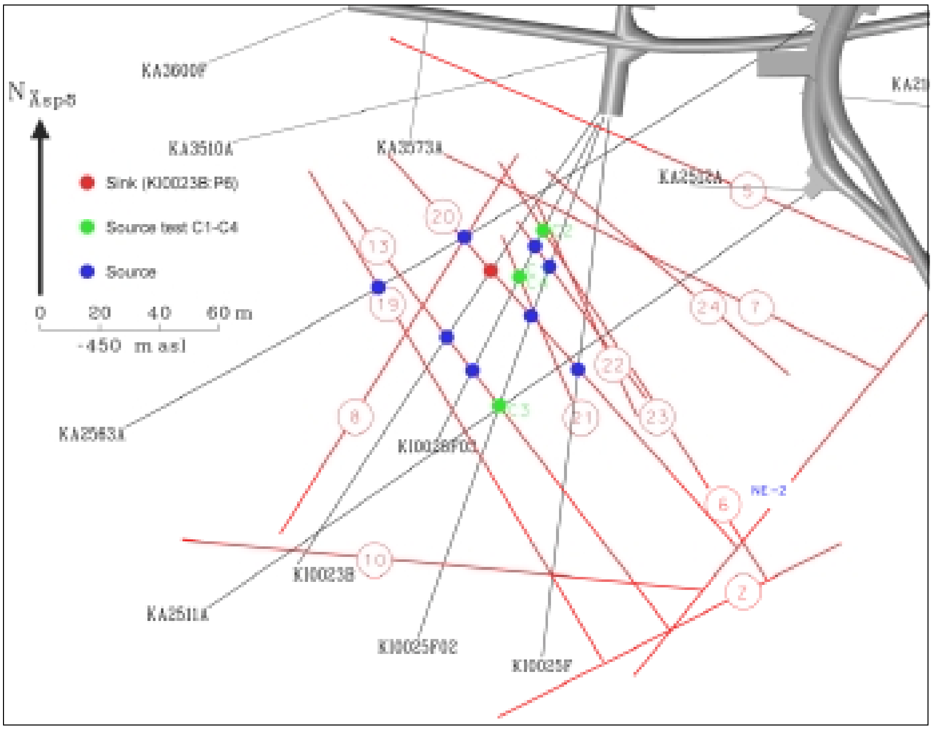


***Figure 4-1.** Overview of the experimental geometry and packer locations for tracer tests using KI0023B:P6 as sink (flow paths I–XI). Position of sinks and sources are related to borehole intersections with the numbered structures and therefore represent different depths.*

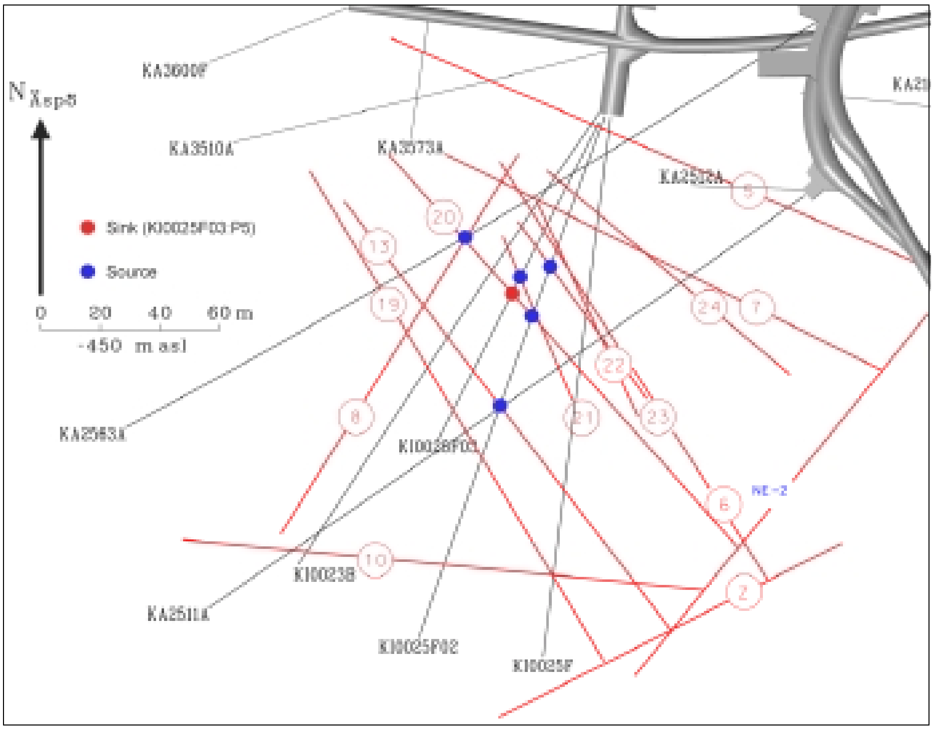


***Figure 4-2.** Overview of the experimental geometry and packer locations for tracer tests using KI0025F03:P5 as sink (flow paths XII–XVI).*

4.2.1 Flow paths within Structure #20

Six flow paths have been tested within Structure #20 (I, VI, IX, XI, XIII and XVI) which cover distances between 11 and 47 m /Andersson et al, 2002b/. Despite the fact that Structure #21 is involved in some of these flow paths they are interpreted to be dominated (90% in terms of length) by transport in Structure #20 and are hence referred to as single structure flow paths. Some flow paths have been run across fracture intersections with Structure #21 and #22, cf Table 4-1.

Path I (14 m long) was identified as the best suited for tests with radioactive sorbing tracers (high mass recovery and short travel time). This flow path has been tested at five different occasions, at different sink strengths, and using different types of injection procedures. The difference in shape of the breakthrough curves in the latter case indicated that different, or partly different physical flow paths in fact had been activated. A test performed at a reduced flow rate showed a delayed and broader peak in the breakthrough. By theory the tail of the breakthrough affected by diffusion should exhibit a slope of –3/2 in a log-log diagram. The slopes of the breakthrough curves obtained for the TRUE Block Scale tests carried out in Path I (Structure #20) generally are steeper (about –5/2) but are less steep than would be expected from pure advection-dispersion, cf Figure 4-3. Type families of breakthrough curves for all six investigated flow paths in Structure #20 are shown in Figure 4-4.

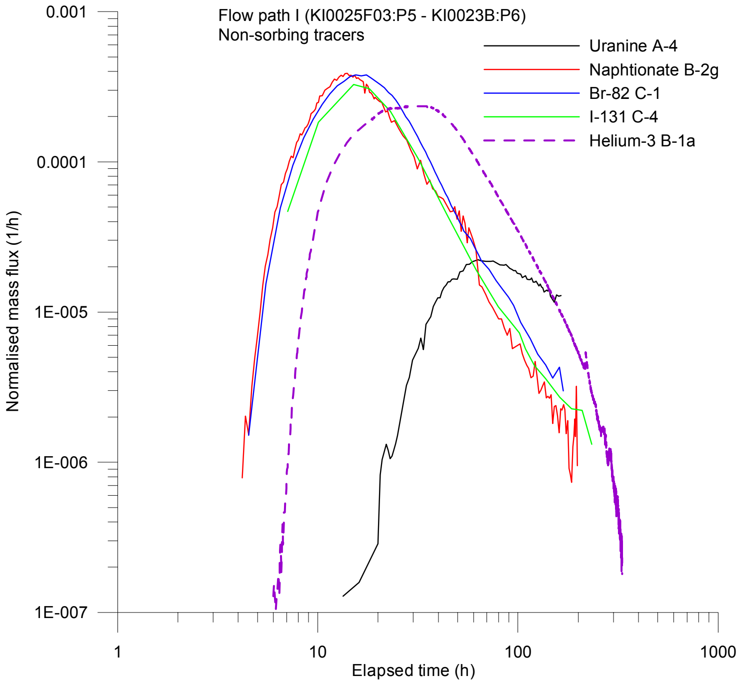


Figure 4-3. *Flow path I – Normalised tracer breakthrough curves for conservative tracers during tests A-4 (passive injection), B-1a (Helium, a tracer with higher diffusivity), B-2g, C1 and C4.*

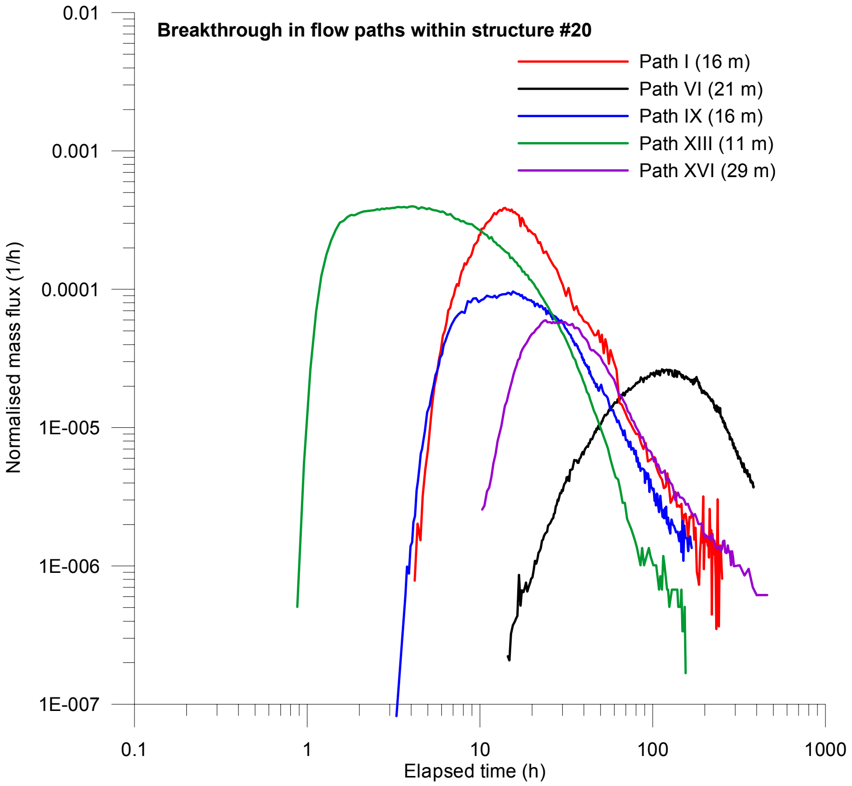


Figure 4-4. *Comparison of tracer breakthrough for conservative tracers in five different flow paths within Structure #20.*

4.2.2 Flow paths in Structure #21

Two flow paths, 33 m (III) and 27 m (V) long, respectively, cf Table 4-1, were tested with approximately the same orientation along the structure. Of particular interest is the relatively long flow path III (L=33 m) which was used later for tests with radioactive sorbing tracers. Flow path III tests show indications of possible channelised flow (non-linear changes in travel time and increased apparent dispersivity in response to reduced pumping rates).

A comparison between conservative experiments run in the two single structure flow paths indicate that transport in Structure #20 is fast and, overall, less affected by diffusion effects than observed for transport in Structure #21. Tests in both of the single structures are to a variable degree affected by other global sinks, in some cases interpreted to be possibly related to fracture intersection effects (reduced mass recovery).

4.2.3 Network flow paths

Of the 8 tested network flow paths only six produced measurable conservative breakthrough within the sampling periods (220–640 hours) assigned for the tests. Four of the remaining flow paths used KI0023B:P6 as sink and the remaining two used KI0025F03:P5, cf Table 4-1. One of these flow paths, Path II, featured by a high mass recovery (88%) and possible involvement of as many as 4 structures, cf Figure 4-2, was selected for injection C2 of radioactive tracers as part of Phase C. A general observation for this flow path is that the travel times and dispersivities generally are low in relation to the projected flow path distances along the structures of hydrostructural model. This may be a possible indicator that the actual *in situ* flow path in fact is shorter than projected, and that the flow path may involve other structures/fractures (yet unknown, or part of the background fracture population). Generally, the longer flow path lengths, cf Table 4-1, entails lower mass recoveries (< 60%), again partly attributed to **fracture intersection effects**. All network flow paths show less steep tailings in log-log plots of the breakthrough curves, compared to those observed in Structure #20. Those flow paths which did not show a breakthrough within the allotted sampling times, X and XII, are in both cases interpreted to be due to lack of, or very low, connectivity.

The probable causes for the low mass recovery (< 70%) noted for some of the flow paths, whether single structure flow paths or network flow paths, are many. In the following list, probable causes for low mass recovery are listed;

- background flow carrying tracer mass to another sink (e.g. the main access tunnel),
- irreversible sorption,
- tracer degradation (biological or physical),
- exchange with stagnant zones along the flow path,
- “dilution” (parts of the mass below detection limit),
- too short sampling time (test duration),
- enhanced diffusion/sorption in fracture rim zone,
- enhanced diffusion/sorption in fine-grained fault gouge.

4.2.4 Experimental evidences of *in situ* retention

The last phase of the TRUE Block Scale Tracer Test Stage, Phase C, was devoted to tests with radioactive sorbing tracers with the purpose to study the retention characteristics and evaluating the retention properties of the selected flow paths. Three flow paths showing high tracer mass recovery – I, II and III (Table 4-1) – were selected for these tests. The three selected flow paths have different characteristics; Path I being primarily a **fast single-structure flow path** within Structure #20, Path II being a **“network” flow path** with transport within Structures #23, #22 and #20, and Path III being an interpreted **long single structure flow** path within Structure #21. Thus, this selection would enable study of differences in retention properties between two single structure paths and a network path. A detailed description of the performance of the tests and their interpretation is presented by /Andersson et al, 2001c, 2002b/.

Some **basic conclusions** can be drawn from the **relative appearance of the breakthrough curves** even without resorting to simple models /Andersson et al, 2001c, 2002b/ or complex numerical simulations /Poteri et al, 2002/ . Results from Path I (C1/C4) shows breakthrough for all injected tracers but one (Zn being the exception) (Figure 4-5). It is also noted that the retention seen in the C1/C4 experiment (transport length of ~14 m with an average transport time of ~18h) is comparable with that observed in the TRUE-1 experiments on a 5 m length scale /Winberg et al, 2000; Andersson et al, 2002b/. For the longer flow paths studied – injections C2 and C3 – no breakthrough was detected for the moderately and strongly sorbing tracers used (i.e. Ba^{2+}, Rb^{+} and Cs^{+}). It is noted that for studies of longer flow paths with geological, structural and hydraulic conditions similar to those met at the TRUE Block Scale site, it appears that only slightly sorbing tracers (i.e. Na^{+}, Ca^{2+} and Sr^{2+}) can be used in an informative way over the time period investigated (< 3300 hours, equivalent to the "official" monitoring period of the project).

The basic modelling evaluation presented by /Andersson et al, 2001c, 2002b/ makes use of a one-dimensional advection-dispersion model where dispersivity and mean travel times were determined using an automated parameter estimation. Specifically, in the case of the Phase C tests a one-dimensional advection-dispersion model with matrix diffusion and sorption was employed. The parameters governing diffusion and sorption are in this case lumped into the so-called *A*-parameter, cf /Andersson et al, 2002b/ that incorporates hydrodynamic effects on retention as well as diffusion/sorption and surface sorption.

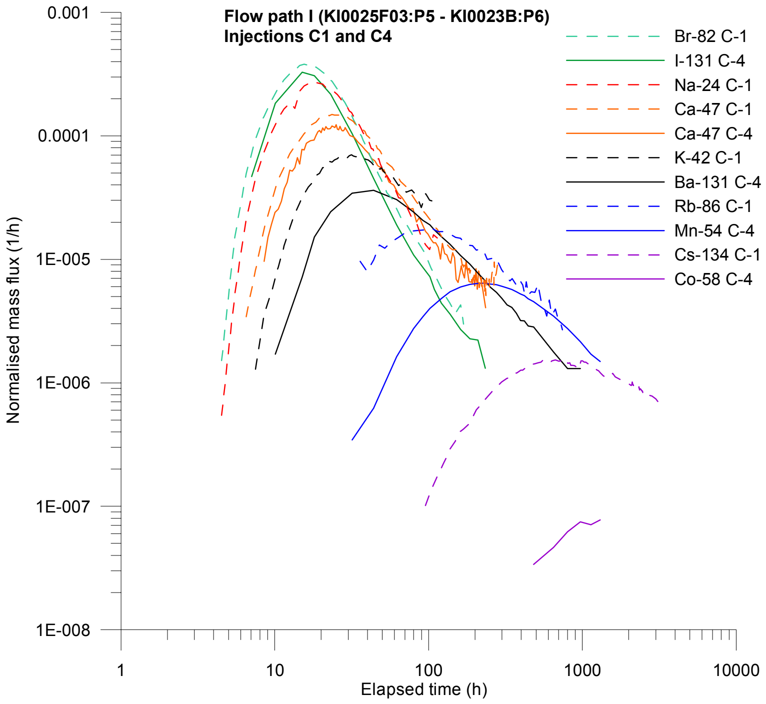


Figure 4-5. *Normalised tracer breakthrough for all tracers injected in tests C1 and C4.*

5 Major modelling accomplishments

Numerical modelling has constituted an important and integrated component in the successful performance of the TRUE Block Scale Project. Early on in the project (Scoping and Preliminary Characterisation Stages), modelling was restricted to Discrete Feature Network modelling (DFN). During the Detailed Characterisation stage additional **modelling concepts** were added – Stochastic continuum (SC) and Channel network (DFN/CN) models). Modelling efforts culminated during the Tracer Test Stage and Evaluation and Reporting Stages with **model predictions** of the tracer tests performed with radioactive sorbing tracers and subsequent model evaluation, partly steered by the formulated hypotheses, cf Section 1.6. In these last modelling efforts two additional concepts were added, namely the LaSAR concept /Cvetkovic et al, 1999/ extended to the block scale and the so-called Posiva streamtube approach /Hautojärvi and Taivassalo, 1994/. To these five concepts should also be added the 1D advection dispersion approach used by SKB-Geosigma for the **basic evaluation of each tracer test**, cf Section 4.2.4 /Andersson et al, 2002b/. It is beyond the scope of this report to account for the detailed theory and methodology of all the different approaches. Details are provided by /Poteri et al, 2002/ and /Winberg, 2001/. However, the **unifying transport theory** considered as part of the project, and which links all the transport approaches used, is presented in Section 5.5.

The **modelled domain sizes** were for the most part in the order of 500x500x500 m, in some cases with more detail (inclusion of background fractures in DFN/CN model) added to an inner 150x150x150 m model. **Boundary conditions** were collected from available numerical site scale models, SC /Svensson, 1997/ or DFN /Holton, 2001/.

The assembly of different model concepts available for the final phases of model prediction and evaluation /Poteri et al, 2002/ constitute a wide spectrum and contain model approaches which could be tentatively labelled as **site characterisation models** (SC, DFN and DFN/CN). This implying that the approaches could be also used as part of the evaluation of a potential repository site. The remaining two concepts are potentially applicable to repository performance assessment (LaSAR and Posiva streamtube approaches). The Posiva streamtube approach has been employed in the most recent Finnish safety analysis. The Posiva TILA-99 migration calculations /Vieno and Nordman, 1999/ were done in two parts: WL/q estimates using continuum and DFN groundwater flow models and migration (retention) calculations using “streamtube” and estimated values of WL/q, cf definition in Section 5.5.

5.1 Scoping and experimental design

The original intention of the project was to prepare numerical simulations of the hydraulic responses of the studied block each time the hydrostructural model was updated, and to use the model results to design the next step of characterisation activities. Due to the relative immaturity of the early hydrostructural models it is really only in conjunction with drilling of the last two boreholes (KI0025F02 and KI0025F03) that useful results could be generated. This is also in accord with the findings from the evolution of hydrostructural models /Andersson et al, 2002a/ where the important characteristics of the investigated rock block were captured by the first three boreholes and associated characterisation (KA2563A, KI0025F and KI0023B). In particular, the last borehole, KI0025F03, was subject to elaborate design calculations to facilitate optimal coverage of source sections for tracer tests with various objectives.

5.2 Prediction of reactive tracer tests

During the TRUE Block Scale experiment, modelling groups were asked to provide predictions on the outcome of reactive tracer tests given the results of conservative tracer tests along the same flow paths. The majority of the modelling groups involved (JNC-Golder, Posiva-VTT, Nirex-Serco and SKB-WRE) had prior experience in modelling solute transport related to Äspö conditions. The ENRESA-UPV/UPC modelling lacked this site-specific Äspö experience.

Although a defined data set for model prediction was provided prior to the predictions (part of Chapter 7 in /Andersson et al, 2002a/) the modelling groups were free to use their own experience and judgement is selection of the parameters that would go into the model predictions. Some groups decided to use the laboratory data provided relating to TRUE Block Scale, and some groups decided to use the MIDS data set provided for TRUE-1 /Winberg et al, 2000/. Furthermore, based on the similarities between the investigated TRUE-1 “Feature A” and the investigated structures in the TRUE Block Scale rock volume, one group (SKB-WRE) used their evaluated *in situ* retention parameters from TRUE-1 for the prediction of the TRUE Block Scale Phase C experiments.

The modelling groups were also given access to the results of the cross-hole interference tests, tracer dilution tests and results of relevant non-sorbing tracer tests performed in the flow paths at relevant pump rates (from Phases A and B). They were then asked to **predict the reactive tracer breakthrough** and **associated mass recovery** of the Phase C tests.

Tables 5-1 through 5-3 show the predicted arrival times for 5%, 50% and 95% of the tracer mass in C1, C2 and C3, as well as the mass recovery as predicted by the 5 modelling teams. The tables also provide a **comparison with** the actual ***in situ* test results** for the Phase C tests including *in situ* mass recovery given at the termination of “official” sampling for Phase C. The measured mass recovery should not to be regarded as final, since some tracers kept arriving after the last measurement was made.

The predicted and measured breakthrough and cumulative mass arrivals are plotted in Figures 5-1 through 5-15, jointly with measured breakthrough. For SKB-WRE the results related to evaluated *in situ* retention parameters from the TRUE-1 analysis are shown. In the figures, the presentation of "measured *in situ* data" is limited to what had been detected at the end of the first stage of the TRUE Block Scale project (t< 3300 hours). *In situ* monitoring was continued thereafter, so the curves for some of the most reactive tracers will be completed/updated as part the continuation of the project. Specifically, some of the more reactive tracers injected during tests C2 and C3 had not yet been detected when the last measurement presented herein was collected. This does not imply that these tracers will never show up. Also, not all tracers were studied by all modelling groups.

A quick overview of the figures clearly shows **block scale reactive transport adds a significant "spread" in the range of predictions** among the different modelling approaches. This spread becomes more pronounced with increasing path length (C2 and C3). The results for C1 in terms of bromide (Figure 5-1), show predictions which are in the same range. For K (Figure 5-4), Rb (Figure 5-5) and Cs (Figure 5-6), the differences in predictions span more than an order of magnitude. What should be remembered is that the conditions applicable to flow path I and the C1 injection very much resemble those met in the TRUE-1 experiments; the distance is in the same order and in addition there exists a geological and mineralogical similarity between Structure #20 of C1 and Feature A investigated as part of the TRUE-1 tests.

In the case of the C2 and C3 predictions, the span in terms of peak arrival is more than an order of magnitude, cf Figures 5-7 through 5-10 and 5-11 through 5-15, respectively.

Two kinds of differences may explain the range of responses obtained by the groups: On the one hand, assuming that the differences between the conceptual models employed by the groups are unimportant, the variations in modelled responses must be due to the use of widely varying input parameters, cf /Poteri et al, 2002/. On the other hand, if variations in responses do not appear consistent with the magnitudes of the parameters used by the groups, then they must be due to the differences in the conceptual models (including description of flow) employed by the modelling teams.

A full comparison of the prediction results of the modelling teams in relation to the input has to take into account the assigned retention parameters and the underlying conceptualisation of the system (flow field and micro-structure/immobile zones). To the extent that models with similar input data produce comparable output, the underlying conceptualisation of the flow field and description of immobile pore space (number of immobile zones, geometry and parameter values) produce a net effect which is nearly the same. In Section 5.6, attempts are made to evaluate the relative effects of the flow field on the evaluated retention.

Table 5-1. Measured and predicted characteristic times and recoveries for the C1 injection. Times T_{xx} in hours, Recovery in % of total injected mass.

Tracer	Measure	Measured	ENRESA	JNC	Nirex	Posiva	SKB
Br-82	**T_5**	9	7.5	11	8	10	8.5
	T_{50}	20	16.5	26	12.4	43	23
	T_{95}	49	31.5	131	23.4	5638	157
	Recovery	100 (160h)	100	100	100	96	95
Na-24	**T_5**	10	9	11	8.8	13	8.1
	T_{50}	27	23	24	12.1	37	20.5
	T_{95}	110	37	121	23.1	0	146
	Recovery	96 (110h)	100	100	100	94	93
Ca-47	**T_5**	14	10	11	9.8	25	8.8
	T_{50}	46	26	26	12.7	197	23.6
	T_{95}	260	65	131	25.5	0	333
	Recovery	98 (300h)	100	100	100	88	95
K-42	**T_5**	21		320	9.4	37	36
	T_{50}	100		750	13	645	377
	T_{95}	D		0	25.5	0	0
	Recovery	53 (110h)		92	100	80	23
Rb-86	**T_5**	66	34	45	40	196	77
	T_{50}	400	110	104	48	5048	779
	T_{95}	D	330	660	68	0	0
	Recovery	67 (730h)	100	99	100	59	49
Cs-134	**T_5**	530		160	85	1227	1072
	T_{50}	5000		450	103	0	11270
	T_{95}	0		2600	139	0	0
	Recovery	39 (3255h)		97	100	41	23

D=Short-lived isotope that had decayed before the specified mass recovery could be reached.

Table 5-2. Measured and predicted characteristic times and recoveries for the C2 injection. Times T_{xx} in hours, Recovery in % of total injected mass.

Tracer	Measure	Measured	ENRESA	JNC	Nirex	Posiva	SKB
Re-186	**T_5**	94	60	74	436	67	73
	T_{50}	260	180	200	568	263	191
	T_{95}	D	438	0	0	0	6211
	Recovery	80 (500h)	100	73	73	93	74
Ca-47	**T_5**	300	105	123	324	335	81
	T_{50}	D	330	370	380	6324	241
	T_{95}	0	750	0	0	0	9428
	Recovery	29 (800h)	100	66	86	61	78
Ba-131	**T_5**	0		850	442	1715	642
	T_{50}	0		0	572	0	4872
	T_{95}	0		0	0	0	0
	Recovery	0 (1900h)		7	79	33	27
Cs-137	**T_5**	0		0	2041	0	40136
	T_{50}	0		0	3390	0	4E+05
	T_{95}	0		0	0	0	0
	Recovery	0 (3197h)		0	91	1	0

D=Short-lived isotope that had decayed before the specified mass recovery could be reached.

Table 5-3. Measured and predicted characteristic times and recoveries for the C3 injection. Times T_{xx} in hours, Recovery in % of total injected mass.

Tracer	Measure	Measured	ENRESA	JNC	Nirex	Posiva	SKB
HTO	**T_5**	230	175	145	70	155	154
	T_{50}	820	0	330	118	953	441
	T_{95}	0	0	2000	298	0	14729
	Recovery	73 (3050h)	42	96	100	83	86
Na-22	**T_5**	340	190	152	73	301	154
	T_{50}	1500	0	380	147	3886	448
	T_{95}	0	0	0	0	0	15327
	Recovery	70 (3100h)	41	82	100	67	86
Sr-85	**T_5**	640	200	164	71	731	172
	T_{50}	3000	0	370	123	0	538
	T_{95}	D	0	1600	303	0	20066
	Recovery	52 (3100h)	44	99	100	47	83
Rb-83	**T_5**	0		500	352	0	6964
	T_{50}	0		1400	466	0	58857
	T_{95}	0		0	695	0	0
	Recovery	0 (3219h)		86	100	2	0.4
Ba-133	**T_5**	0		1100	114	5798	1538
	T_{50}	0		0	178	0	11526
	T_{95}	0		0	371	0	0
	Recovery	0 (3219h)		8	100	13	19

D=Short-lived isotope that had decayed before the specified mass recovery could be reached.

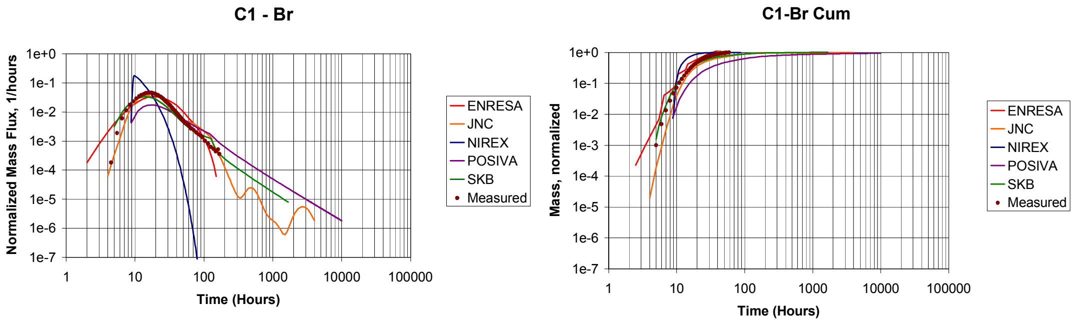


Figure 5-1. Predicted and measured breakthrough curves for Bromide, test C1.

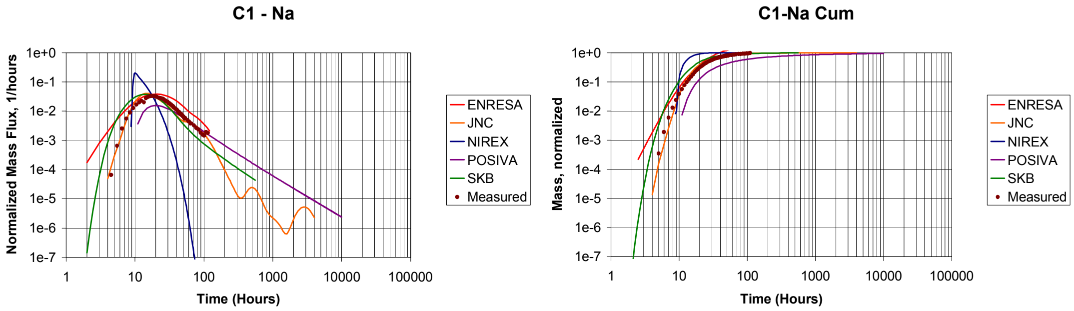


Figure 5-2. Predicted and measured breakthrough curves for Sodium, test C1.

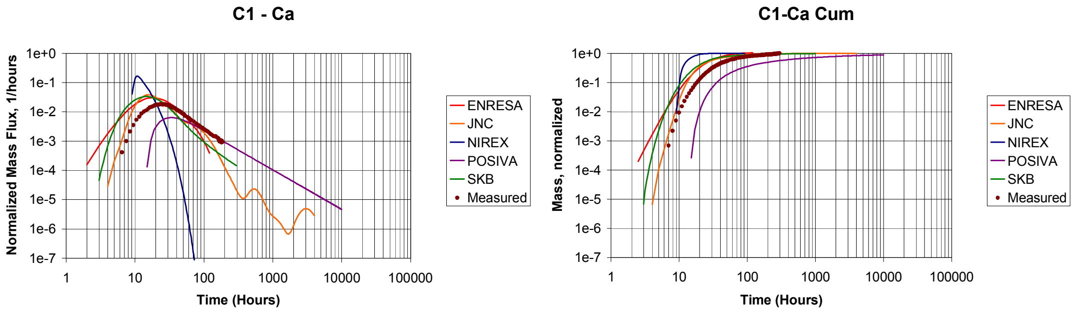


Figure 5-3. Predicted and measured breakthrough curves for Calcium, test C1.

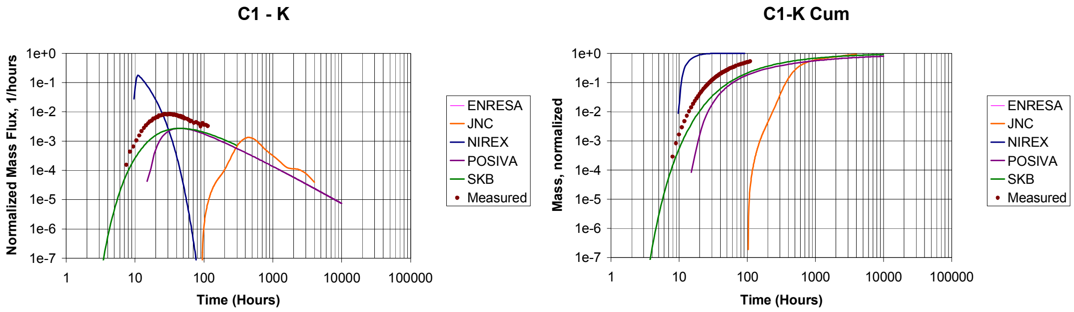


Figure 5-4. Predicted and measured breakthrough curves for Potassium, test C1.

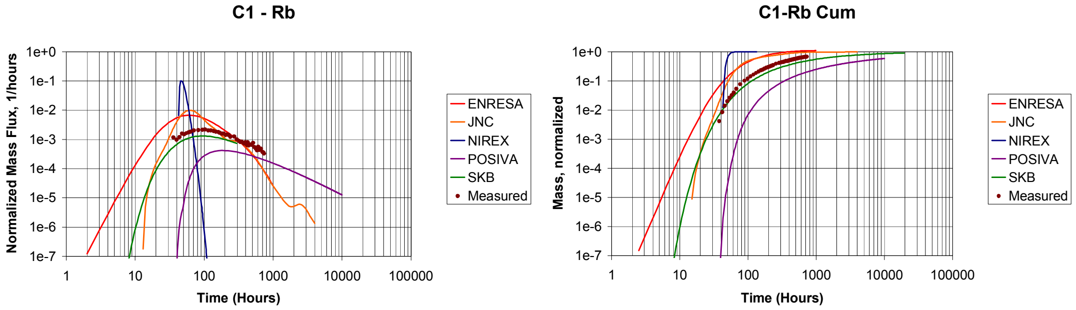


***Figure 5-5.** Predicted and measured breakthrough curves for Rubidium, test C1.*

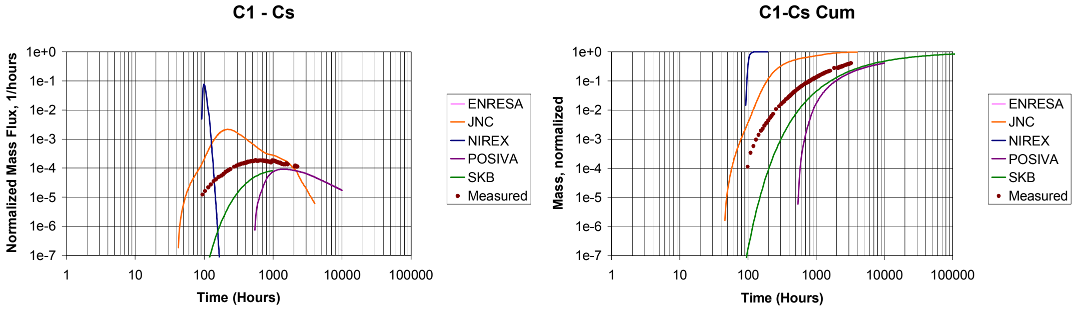


***Figure 5-6.** Predicted and measured breakthrough curves for Cesium, test C1.*

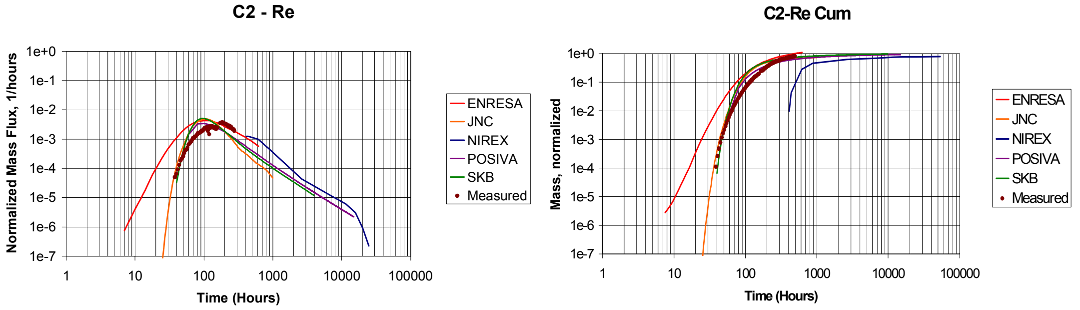


***Figure 5-7.** Predicted and measured breakthrough curves for Rhenium, test C2.*

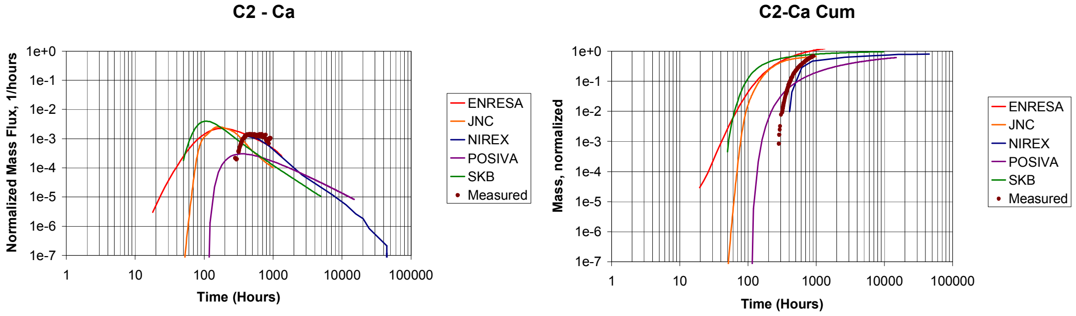


***Figure 5-8.** Predicted and measured breakthrough curves for Calcium, test C2.*

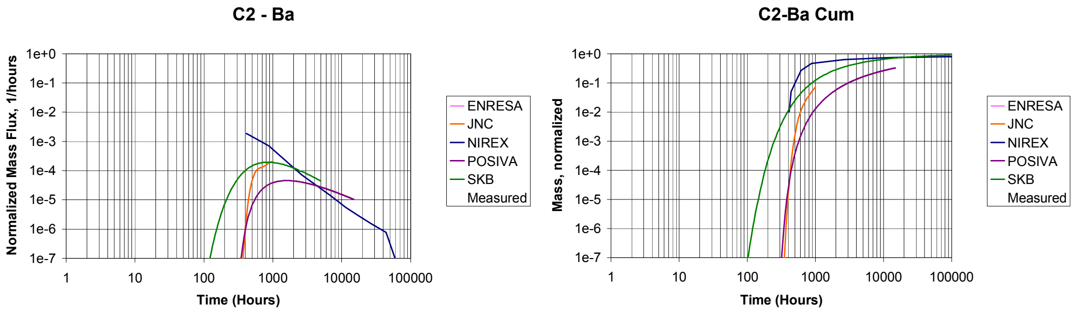


Figure 5-9. Predicted and measured breakthrough curves for Barium, test C2.

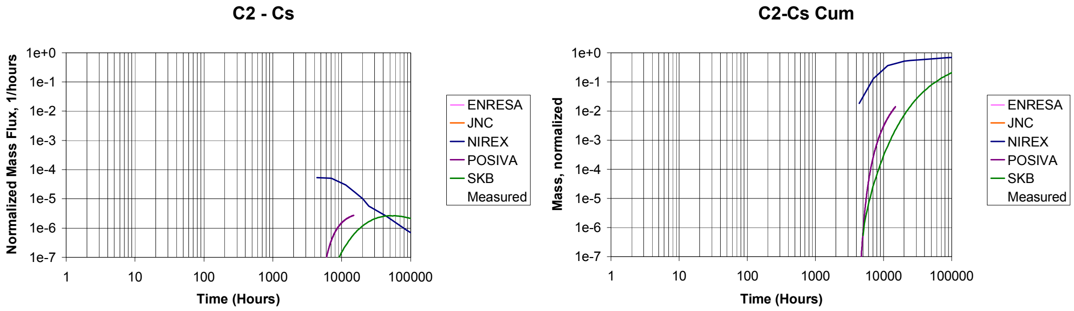


Figure 5-10. Predicted and measured breakthrough curves for Cesium, test C2.

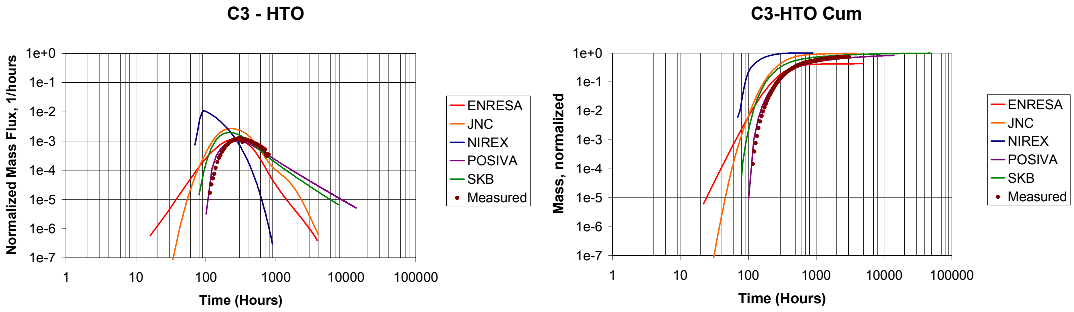


Figure 5-11. Predicted and measured breakthrough curves for tritiated water, test C2.

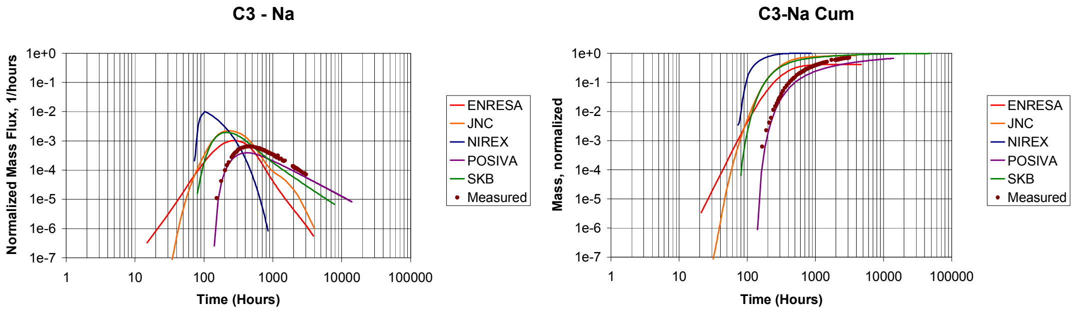


Figure 5-12. Predicted and measured breakthrough curves for Sodium, test C3.

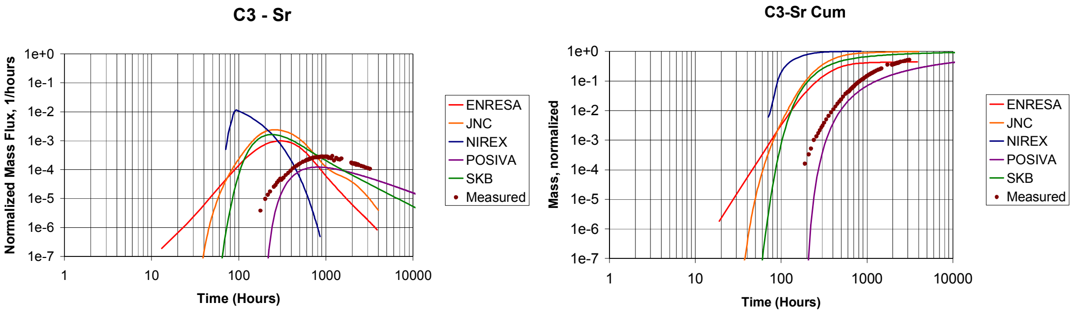


Figure 5-13. *Predicted and measured breakthrough curves for Strontium, test C3.*

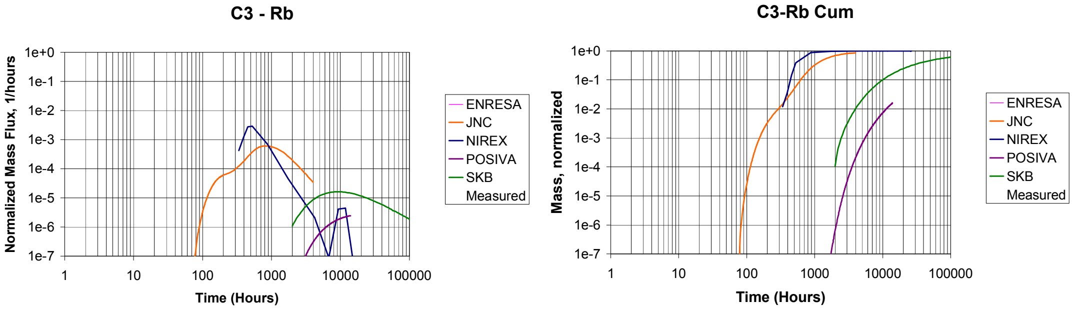


Figure 5-14. *Predicted and measured breakthrough curves for Rubidium, test C3.*

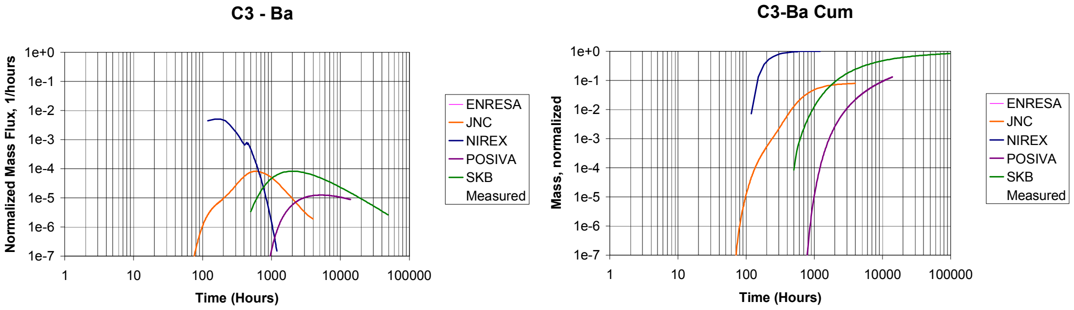


Figure 5-15. *Predicted and measured breakthrough curves for Barium, test C3.*

5.3 Testing of hydrostructural model (Hypothesis 1)

Testing of the hydrostructural model has primarily been carried out with two models/approaches – the stochastic continuum /Gómez-Hernández et al, 2002/ and channel network models /Dershowitz and Klise, 2002; Rachez and Billaux, 2002/, cf /Poteri et al, 2002/ for a summary.

The former modelling approach describes the fractured rock mass as a heterogeneous continuum. The flow model is stochastic which enables generation of alternative **realisations** of the studied rock block, which are consistent with the available data. The modelled volume is divided into equally sized cells over which the information of the hydrostructural model is superimposed. Cells intersected by a deterministic

structure were assigned hydraulic conductivity values according to intersecting structures, and vice versa. An underlying assumption is that a non-negligible fraction of transport occurs in the rock mass. The flow model is calibrated on hydraulic conductivity, hydraulic head (static head and transient from cross-hole interference tests) resulting in **calibrated conductivity fields and boundary conditions**.
By comparing an initial realisation (calibrated only to conductivity) with the final conditioned realisation (static head plus transient head data from hydraulic tests) it was possible to identify which of the interpreted deterministic structures that become more permeable, and which become less permeable. Initially, all interpreted deterministic structures were assigned a logK (m/s) of –6.5. Analysis of the October 1997 model /Andersson et al, 2002a/ indicated an increase in the logK of the northeast Structure #8 and subhorizontal Structure #16 by more than an order of magnitude. Similarly, the log K of Structure #5 increased by two orders of magnitude. The latter is in accord with the hydraulic understanding of the site. However, both Structures #16 and #8 are considered as hydraulically insignificant from available borehole and tunnel data. Hence, a need to look for more of a north-south hydraulic connection through the block was identified. A careful scrutiny of available data subsequently resulted in upgrading of three fractures belonging to the background fracture population to become deterministic Structures #21–#23, cf Figure 2-1. These structures provided the required geological explanation for the interpreted more north-south hydraulic connection /Andersson et al, 2002a/. Additional verification of these structures was provided through drilling and characterisation of borehole KI0025F03.

The channel network model /Dershowitz and Klise, 2002/ was used to test the hydrostructural model in two contexts. The first includes definition of **typical pressure response patterns of fracture networks** and comparing type responses to those observed in the performed field tests. The second includes **comparison between** the **simulated and observed *in situ* drawdowns**. The typical response patterns in distance-drawdown graphs (s/Q vs t/R^2) were divided into the following four classes (cf /Poteri et al, 2002/ for details and exemplification);

1. **Network Response:** The greater the distance from the hydraulic source, the weaker the response. This is the classic distance-drawdown response.

2. **Compartment Response:** All points respond approximately the same, regardless of the distance from the hydraulic signal. This typically occurs within single structures of high transmissivity, with poor connection to hydraulic boundary conditions.

3. **Flow Barrier Response:** Points show little or no hydraulic response, regardless of the distance from the hydraulic signal. This can be due to a lack of hydraulic connection, or due to a strong connection to a constant head boundary condition.

4. **Heterogeneous Response:** Responses are observed which are only poorly correlated to the Cartesian distance. This response is typical of cases where there are strong conductors, which are connected to the hydraulic source and some of the monitoring sections, but are not connected into the overall fracture network.

A scrutiny of available responses in the above context and a corresponding comparison with simulation results from the DFN/CN model is provided in Table 5-4. Interestingly, the **predominant *in situ* response pattern is** a **compartmental** response. This is **inconsistent with the hydrostructural model** that provides extensive connections. The level of connectivity of the hydrostructural model is evident in the fact that the DFN/CN model simulations based on the hydrostructural model show network responses, even for a DFN/CN model without background fractures.

The **too high connectivity in the hydrostructural model** is evident also in the simulated DFN/CN drawdowns being significantly smaller those observed *in situ*. This implies that the DFN/CN model is better connected to the boundary conditions than the *in situ* rock mass. It was demonstrated /Poteri et al, 2002/ that the comparison between the model results and the *in situ* measurements could be improved somewhat by;

- Breaking up Structure #21 in segments to reduce over-connectivity (this action compatible with geological observation).
- Low permeability zones have been added for the fracture intersection zones between Structures #13 and #21 to reduce connectivity (could be explained geologically by barrier effect of fault gouge).
- Transmissivity of Structures #6, #13, #19, #20 and #21 was reduced.

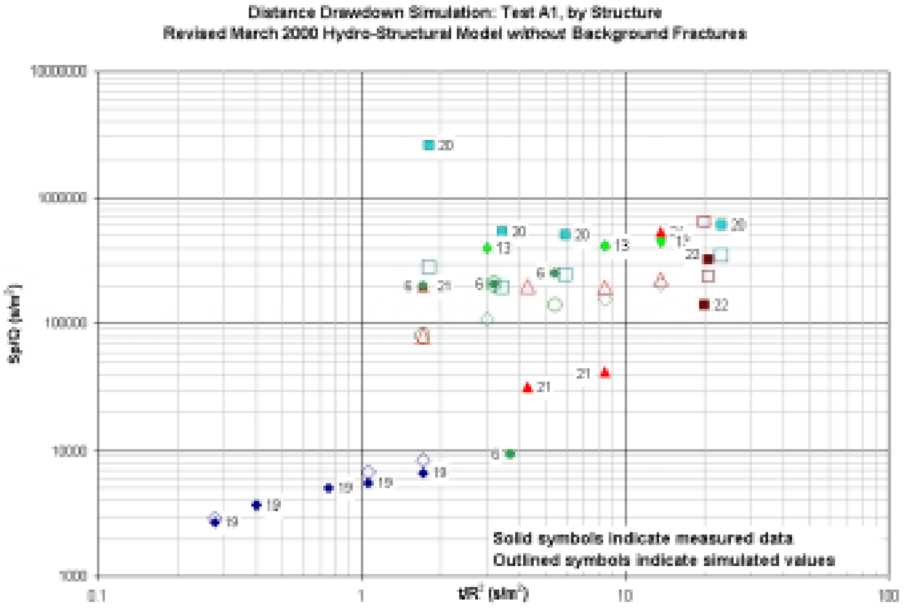
The effect of the above actions is visualised in Figure 5-16.

Table 5-4. Hydraulic responses - experimental data and simulation results from DFN/CN model /Poteri et al, 2002/.

Test	**Sink Structure**	**Network response** – Experimental – *Simulation*	**Compartment response** – Experimental – *Simulation*	**Flow barrier response** – Experimental – *Simulation*	**Heterogeneous response** – Experimental – *Simulation*
A-1	20	6, 21	20, 23	5, 19	7, 13, 22
		6, 7, 19, 21	*13, 20, 22*	–	*5, 23*
A-2	21	6	20, 22, 23	5, 19	7, 13, 21
		6, 7, 19, 21	*20, 22, 23*	–	*5, 13*
A-3	20	–	20, 21, 22, 23	5, 19	6, 7, 13
		6, 7, 13, 19, 20	*21, 22, 23*	5	–
A-4	20/21	6, 13, 21	20, 22, 23	5, 19?	7
		6, 7, 19	*20, 21, 22, 23*	–	*5, 13*
A-5	20	6, 21	20, 22	5	7, 13, 19, 23
		7, 19, 22	*6, 21, 23*	*5*	*13, 20*
B-1	20/21	–	6, 20, 22	5, 19	7, 13, 21, 23
		6?, 7, 19, 21	*22, 23*	*5*	*13, 20*
B-2	20/21	19?	6, 7, 22	5	13, 20?, 21, 23
		6, 7, 19, 21	*22, 23*	*5*	*13, 20,*

/Rachez and Billaux, 2002/ provided a test of the evolving hydrostructural model in relation to simulated tracer transport. In a post-experiment model study using a DFN/CN model they showed a significantly better ability for the most recent hydrostructural model to reproduce selected tracer test results compared to models based on the older, less mature model updates.

Additional aspects of testing the hydrostructural model are provided in Section 5.2, where the performed model predictions of the Phase C tracer tests are discussed.



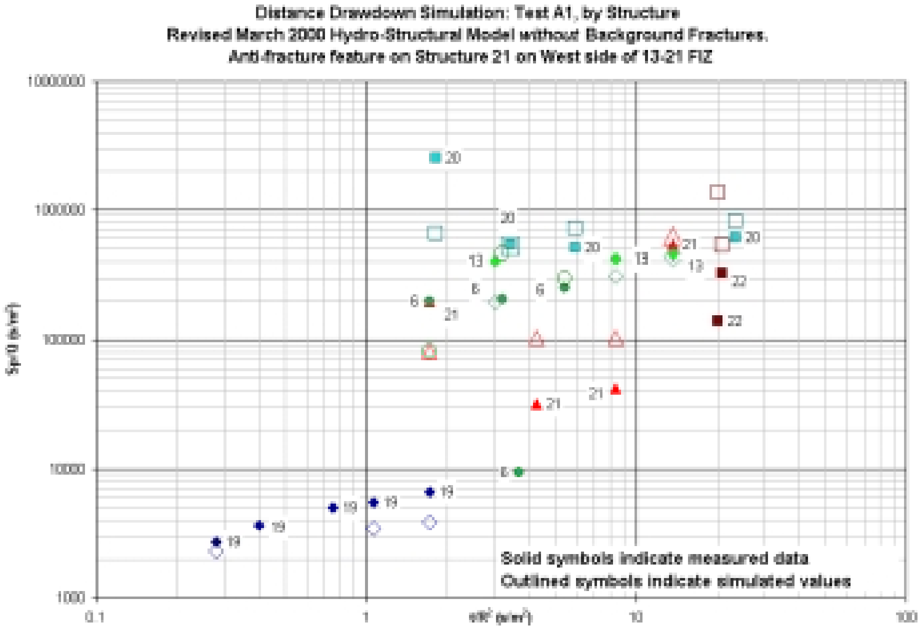


Figure 5-16. *Comparison between simulated drawdown for a) basic hydrostructural model, b) hydrostructural model with imposed changes outlined in accompanying text.*

5.4 Effects of heterogeneity (Hypothesis 2)

Heterogeneity in fractured crystalline rock is a rule rather than an exception. The relative effect of heterogeneity is primarily a question of the **scale of the problem** studied.

On a primary level heterogeneity is introduced by discontinuities on various length scales ranging from discrete minor fractures to major site scale fracture zones. It is also noted that existing discontinuities vary geologically and hydraulically along their extent and may thus differ among borehole intercepts /Andersson et al, 2002a; Mazurek et al, 1997/. In addition, the constitution of the **rock mass** in between discontinuities and the degree and distribution of **infilling materials in the discontinuities** provide additional heterogeneity. A type of heterogeneity added to the block scale is the **fracture intersection zone (FIZ)** which form one-dimensional channels in the rock mass.

Accounting for the heterogeneity of the studied rock block varies among the model approaches and scales. The stochastic continuum flow model included a description of heterogeneity in hydraulic conductivity with an explicit description of spatial continuity both in modelled deterministic structures and in the rock mass (40 m correlation scale). The DFN/CN model accounted for heterogeneity between fractures, but assigned a homogeneous transmissivity to each fracture. Fracture intersection zones were included explicitly in the analysis.

The types of heterogeneity described in the preceding paragraphs are denoted **macro-scale heterogeneity (> 0.1 m)**. The heterogeneity provided by the minute constituents of the fractures/structures (fault breccia and fine-grained fault gouge) and the variability in material transport/retention properties of the chemically-altered wall rock along conductive fractures/structures is referred to as **micro-scale heterogeneity (< 0.1 m).** The macro-scale heterogeneity is the foremost provider of hydrodynamic dispersion.

In the case of transport, attempts were made in the application of the LaSAR approach to include **heterogeneity in micro-scale retention properties** in terms of **porosity variations** on a cm length scale along the modelled flow path and also as an **exponential decreasing trend normal to the fracture surface**. The DFN/CN PathWorks concept provided heterogeneity in transport/retention by dividing the **immobile zones** into three different zones (intact unaltered rock (infinite), altered rim zone and stagnant zone). The Posiva approach treated effects of different immobile zones (matrix rock, fault gouge and stagnant zones) as individual model variations.

In principle, an explicit inclusion of macro-scale heterogeneity and spatial continuity of material properties (hydraulic conductivity/transmissivity) in fractures/structures as well as heterogeneity in micro-scale transport/retention properties is possible within the capability of most of the models employed in the analysis of the TRUE Block Scale experiments. However, for the TRUE Block Scale the amount of micro-scale retention data /Andersson et al, 2002a/ is limited. A full description of these types of heterogeneity, individually (single fracture/structure), or globally for an ensemble of conductive features is not possible. The consequence is that **a statistical description of in-plane hydraulic heterogeneity** and **variability in wall rock porosity**, to a large extent has to be **postulated based on a small number of observations**. This results in description of trends in data, rather than as well-founded statistical correlations, e.g. in terms of a decrease in porosity away from a fracture surface into the intact rock. To partially make up for the paucity of data, data from the neighbouring TRUE-1 site with its similar geological, mineralogical, and geochemical characteristics have been considered /Byegård et al, 1998; Winberg et al, 2000; Byegård et al, 2001/.

In the following, heterogeneity in the description of flow is elaborated upon further. Heterogeneity in transport/retention parameters is addressed in Section 5.6.

Both the DFN/CN model and the SC model made distinctions between the deterministic structures and the **rock mass**. The SC model described the rock mass as a continuum, and the DFN/CN model described the rock mass in terms of a **background fracture population**. The results of the SC model require non-negligible effects of the rock mass between the deterministic structures /Poteri et al, 2002/. Although the mean permeability values of the two populations differ with almost four orders of magnitude there is a clear overlap between the two populations (Figure 5-17). The results from the DFN/CN model on the other hand showed that the addition of a background fracture population actually reduced the performance of the numerical model and worsened the difference between calculated and measured drawdown.

In-plane heterogeneity in deterministic structures was, in the case of the DFN/CN model, introduced at intersections between structures (FIZs). The conclusion of the FIZ-related studies /Winberg, 2000/ was that it was **not possible to observe an influence of the FIZs on the modelled breakthrough**. However, the FIZs could facilitate pathways to alternative sinks in the rock mass resulting in a reduced mass recovery, this has also been observed *in situ*.

In the case of the self-calibrating procedure employed by the SC model, the heterogeneity of both the rock mass and deterministic structures were automatically calibrated to match steady state and transient head data. Through this procedure inconsistencies in the hydrostructural model could be identified, cf Section 5.3. An example of **intra-plane heterogeneity evolved through the process of calibration** is shown in Figure 5-18.

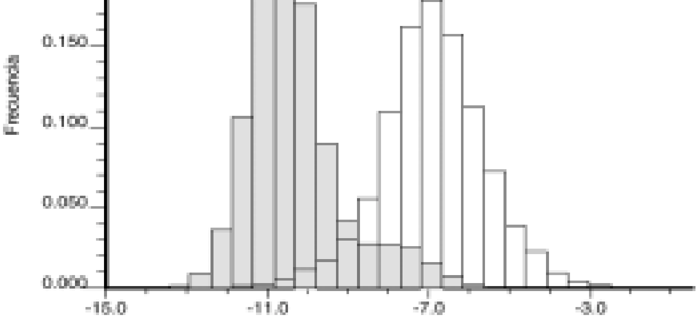


Figure 5-17. *Histograms of log-conductivity (log m/s) obtained from a calibrated realisation, for the rock mass blocks (shaded) and for the blocks defining the conductive structures (white).*

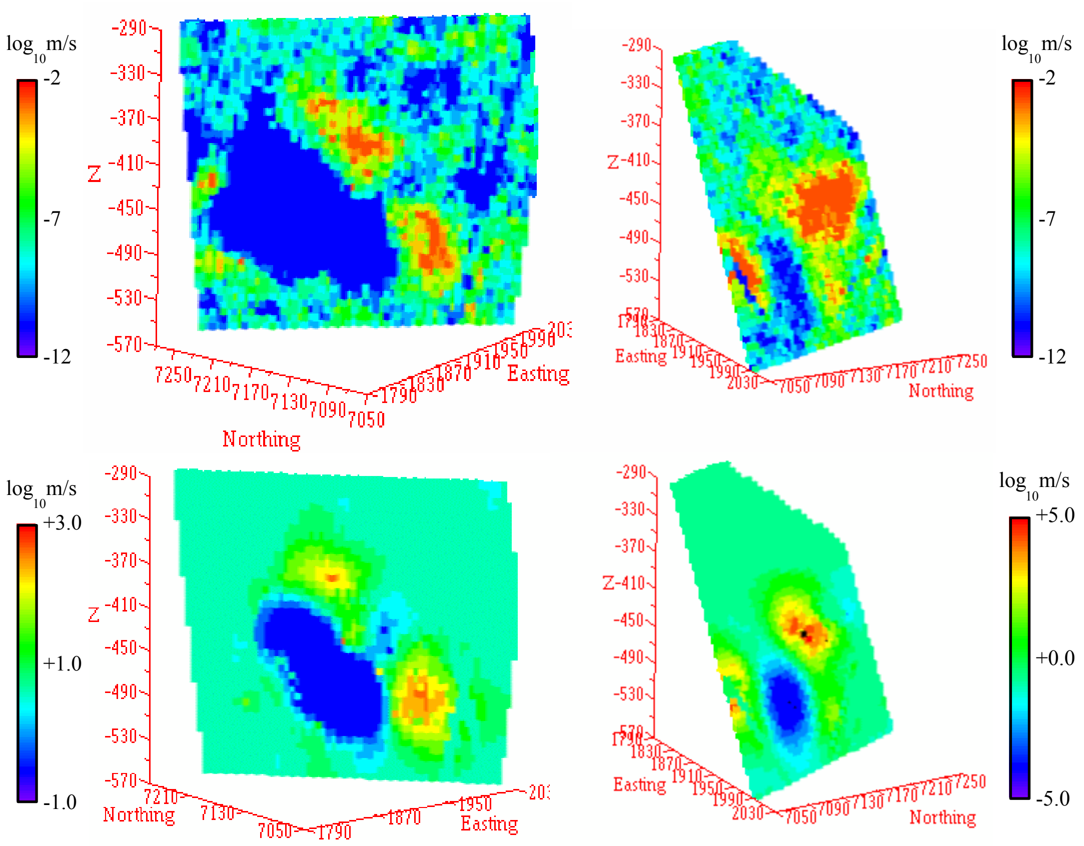


__Figure 5-18.__ Top row: Final distribution of conductivity (log m/s) within Structures #20 (left) and #9 (right) after conditioning to the interference tests. Bottom row: Perturbations applied to the initial conductivity distributions, which were conditioned only to conductivity measurements but not to piezometric head data.

5.5 Common conceptual basis for transport and retention

Crystalline rock is conceptualised as a dual porosity (mobile-immobile) system. Water flows through discrete fractures driven by ambient boundary conditions and is effectively stagnant in the rock matrix. Indivisible tracer particles (e.g. radionuclide ions) enter the flow field at the injection borehole and are transported through one or several fractures to the detection (pumping) borehole. In fractured crystalline rock the **mobile pore space** is primarily the small portion of the total pore space that comprises the void space of the fractures. Water in the remaining majority of the pore space in the rock matrix and fracture filling material is in practice **immobile**. In the TRUE Block Scale experiments the tracer tests are carried out through a network of fractures that provides possibility to study both network effects in advective transport and mass transfer processes between the mobile and immobile pore space.

All TRUE Block Scale modelling approaches consider linear retention, motivated by the fact that TRUE Block Scale tracer tests are sufficiently diluted. As developed by /Poteri et al, 2002/, we can write the *common form* of transport equations used by the TRUE Block Scale modelling teams as;

$$R\frac{\partial C}{\partial t}+V\frac{\partial C}{\partial x}=D_l\frac{\partial^2 C}{\partial x^2}-\sum_{i=1}^{N}\frac{\alpha^i\theta^i D_m^i}{b^i}\frac{\partial C_m^i}{\partial z}\bigg|_{z=0}, \tag{5-1a}$$

and

$$R_m^i\frac{\partial C_m^i}{\partial t}-\frac{\partial}{\partial z}D_m^i\frac{\partial C_m^i}{\partial z}=0 \quad . \tag{5-1b}$$

where C is the solute concentration [ML^{-3}], t is time [T], V is the one-dimensional velocity in direction x [LT^{-1}], D_l is the longitudinal dispersion coefficient [L^{2}T^{-1}], D_m is the pore diffusivity into the rock matrix [L^{2}T^{-1}], C_m is the concentration of the solute in matrix of a retention zone [ML^{-3}], z is the distance normal to the fracture [L], θ is the porosity of the matrix of a retention zone [–], and finally α^i is the fraction of the fracture area in contact with retention zone "i" ($\Sigma\alpha^i = 1$).

Equations (5-1) can, in principle, account for all types of heterogeneity, for which data are available, both in terms of flow and retention. Different modelling teams have used different simplifications of Equations (5-1), different techniques of solution, and different strategies to account for random/deterministic heterogeneity in flow and retention parameters. Details on the different modelling approaches, a more comprehensive discussion of the effects of flow on retention and illustrative typical cases of retention heterogeneity based on the streamtube approach are provided by /Poteri et al, 2002/.

In the following, some key parameter dependencies for advection and retention in crystalline rock are discussed. Equation (5-1) will be simplified such that an analytical solution is available. Tracer particles are assumed to be subject to **two processes**: (i) **advection due to water movement**, and (ii**) retention in the rock matrix and on rock surfaces due to diffusion and sorption**. In other words, retention processes retard particle movements relative to the flowing groundwater. Neglecting dispersion and focusing on plug-flow in a one-dimensional "channel", or streamtube, with the rock matrix as the single retention zone, Equation (5-1) reduces to the retention model for crystalline rock derived from the parallel plate model of /Neretnieks, 1980/, /Carslaw and Jaeger, 1959/, and with dispersion as given by /Tang et al, 1981/ and /Sudicky and Frind, 1982/. It was extended to a heterogeneous fracture by /Cvetkovic et al, 1999/ and to a network of fractures by /Painter et al, 1998/.

Rather than use the homogeneous model of /Neretnieks, 1980/, the parallel plate model is generalised to a series of segments (fractures) in the spirit of /Painter et al, 1998/. The model couples the processes of advection, diffusion and sorption in parallel plate systems in series by the following expressions:

$$\gamma(t,\tau) = \frac{H(t-\tau)B}{2\sqrt{\pi}(t-\tau)^{3/2}} \exp\left[\frac{-B^2}{4(t-\tau)}\right] \tag{5-2}$$

$$B = \sum_{i=1}^{N} \kappa_i \beta_i \quad ; \quad \beta_i = \frac{l_i}{V_i b_i} = \frac{2W_i l_i}{q} \quad ; \quad \tau = \sum_{i=1}^{N} \frac{l_i}{V_i} = \frac{2}{q} \sum_{i=1}^{N} W_i l_i b_i \tag{5-3}$$

$$\kappa_i = \theta_i \left[D_i \left(1 + \frac{\rho_b K_d^i}{\theta_i} \right) \right]^{1/2} \tag{5-4}$$

The solution can be summed up from the piecewise classical solutions (this can be shown easily e.g. in the Laplace domain). In Equation (5-2) surface sorption can be included in τ if desired. The segments can be parts in a single fracture or segments representing several fractures. The total number of segments is N. In (5-2), b [L] is the half-aperture. The parameters θ, D, K_d characterise retention (microscopic) processes. θ [–] is the porosity of the rock matrix, D [L^2/T] is pore diffusivity, K_d [L^3/M] is the partitioning (distribution) coefficient and ρ_b [M^3/L] the bulk density of the rock matrix. The parameter W_i [L] is the width of the flowpath (streamtube) in segment "i". A more comprehensive discussion on the role of b, W and q is provided by /Poteri et al, 2002/.

The function γ (5-2) is in effect a probability density function (pdf) for particle residence time in the network, conditioned on the water residence time τ and on B [$T^{1/2}$]. If there is no retention, then $\gamma(t,\tau)=\delta(t-\tau)$, i.e. particle residence time is equivalent to the water residence time through the fracture network. Tracer discharge into the pumping well is quantified using γ by performing two integrations: first a convolution with the input (injection) function as measured in the injection borehole, and then an integration with the residence time distribution which accounts for hydrodynamic dispersion.

If the retention parameters θ, D and K_d are constant for all segments, we have

$$B=\beta\kappa \quad ; \quad \kappa=\theta\,(1+K_d\,\rho/\theta)^{1/2} \quad ; \quad \beta = \sum_{i=1}^{N} \frac{l_i}{V_i b_i} = \frac{2}{q} \sum_{i=1}^{N} W_i l_i \tag{5-5}$$

The parameter β [TL^{-1}] is dependent only on the water flux distribution, i.e. on fracture hydrodynamics, which in turn is determined by the structure of the network (fractures) and prevailing boundary conditions. For a tracer test where tracer is released from a borehole an estimation of the beta near the source can be made by Equation (5-6) assuming that W_i is approximately equal say to the diameter of the borehole, W_0; then

$$\tau = \frac{2W_0 L b_0}{q} \quad ; \quad \beta = \frac{2W_0 L}{q} \ , \tag{5-6}$$

where b_0 is an "effective" half-aperture for the entire network, q the flow rate through the injection borehole section and $L=\Sigma\, l_i$ is approximately the length of the transport path. In form (5-7), β is assumed to be constant for the whole flow path length and width, and the numerator ($2W_0L$) has been referred to as "flow-wetted surface" by I Neretnieks. An alternative representation of β where we can account for variability within the flow path is a distribution of β's along different (parallel?) trajectories (consistent with hydrodynamic dispersion)

$$\beta = k \ \tau \, , \tag{5-7}$$

where k [L^{-1}] is a parameter to be calibrated on breakthrough data, or independently estimated. Note, that strictly speaking the β's of two streamlines are proportional to the τ's only if the apertures are same. Equation (5-7) should be understood as statistical relationship between β and τ for a large number of streamlines and given boundary/flow conditions.

Ideally, we would like to estimate all *in situ* retention parameters (β, or k, θ, D, K_d for all tracers). From the above expressions, we conclude the following:

- The controlling retention parameter B in (5-2) is an **integrated quantity along the entire flow path**; hence strictly we cannot determine its value from "local" (point) parameter values. This can be done only based on additional simplifications. If microscopic retention parameters θ, D and K_d are assumed uniformly distributed then only β needs to be integrated along the flow path.
- The macroscopic (hydrodynamic) retention parameter β controls retention jointly with the microscopic parameter group, i.e. all the parameters "act" as a group, or product $B=\beta\kappa$. Hence we cannot infer individual parameter values of the group B without invoking **additional constraints,** or independent estimates (i.e. independent of the measured BTCs); we require two constraints (or independent estimates) in order to infer all *in situ* retention parameters.

We can set the two constraints in different ways. One approach is to independently estimate β based either on (i) streamtube approximation, or (ii) Monte Carlo simulations. In the streamtube approach we would use Equation (5-6) with W_0 say the borehole diameter, L the distance between the injection and detection boreholes, and q the flow rate in the injection borehole estimated from dilution tests. The second approach utilises structural and hydrogeological information (obtained from borehole logging, single-hole and cross-hole pumping tests, flow-meter measurements, etc) to construct a statistical discrete fracture network (DFN) model, as has been done by several groups. Monte Carlo DFN particle tracking simulations are carried out and τ and β are computed using (5-3) and (5-5). Based on the generated statistical database, we can establish a correlation between τ and β and in effect infer the slope k in (5-7); given τ, we then have a deterministic relationship for computing β.

Another possible constraint is on the microscopic parameters in form of the so-called Archie's law /Archie, 1942/, which provides a deterministic relationship between porosity and rock diffusivity. Still another possibility, is to use an independent estimate of K_d say from batch experiments on a given size fraction, and assume this value applicable *in situ.*

The above compilation highlights that the **transport modelling approaches** used by the different modelling groups **are conceptually similar**. The main difference lies in which immobile zones that have been invoked, and how they are parameterised, and how heterogeneity has been taken into account.

5.6 Relative role of transport processes (Hypothesis 3)

The TRUE Block Scale Phase C reactive tracer tests were performed using three different injection points and one withdrawal point with separation distances (Euclidean) varying between 14–33 m /Andersson et al, 2002b/. The measured breakthrough curves contain integrated information of *in situ* transport and retention processes active in these tests along the respective flow paths. It is, however, difficult to discriminate different processes based on the breakthrough data alone, because many processes cause similar breakthrough behaviour. Different models used in the evaluation of the tests put emphasis on different characteristics/components of the problem. For this very reason it is advantageous to have parallel modelling efforts using different approaches when evaluating the same *in situ* test data.

The measured breakthrough curves are predicted more or less equally well by different approaches, cf Section 5.2. The advantage is that comparison of the different approaches provides a wider view of retention in solute transport in fractured rock. Different transport and retention processes have different weights in alternative approaches, and this way they can be regarded as **alternative explanations** (hypotheses) to the actual *in situ* retention processes. The comparison is made here through compilations of the parameterisation used by the different approaches to model the tracer tests. Emphasis is placed on the retention processes, not on transport *per se*. In the following we are discussing and exemplifying various aspects of the interplay between different retention processes assumed active during our experiments along the lines of the general formulation of the problem in Section 5.5.

5.6.1 Effects of advection

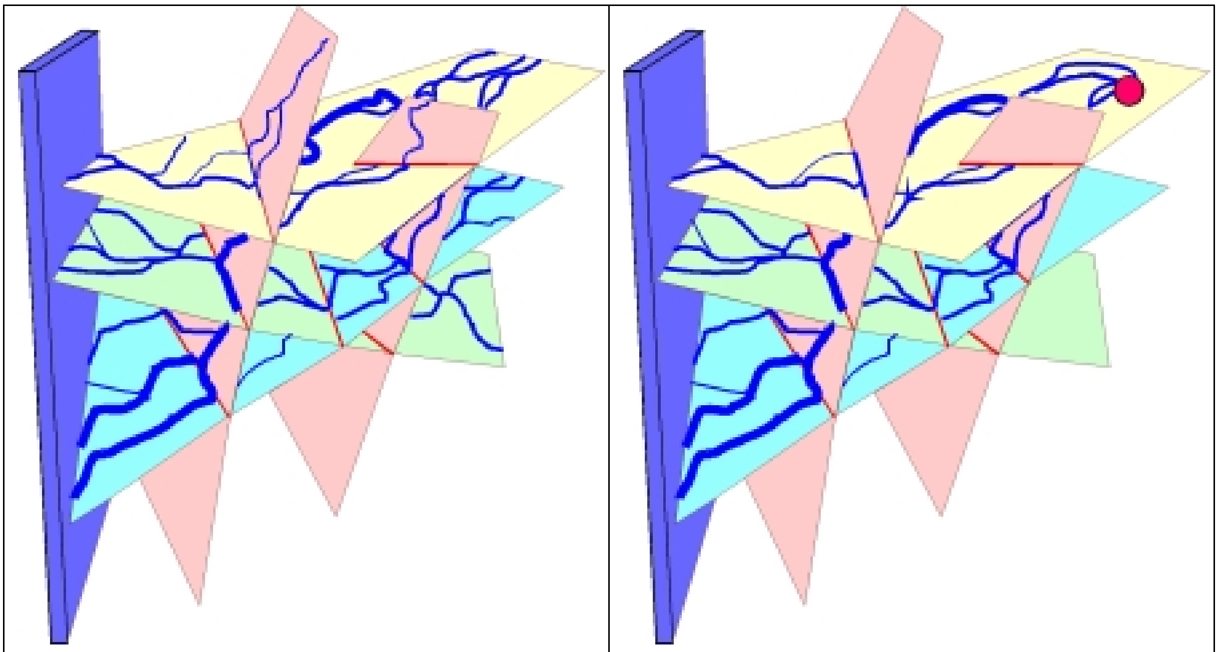
It is clear from Section 5.5 that the **advective flow field** forms a basis, or platform that **determines** the **relative importance of** the different **retention processes**.
In the steady-state flow field, the flow paths of the tracer particles coincide with the streamlines of the flow field. Advective transport is governed by the properties of the streamlines starting from the source and ending at the sink. If no diffusion processes are considered then the transport of the tracer particles is perfectly represented by the streamlines.

The meaning of **heterogeneity** has different meaning in different models. The combined flow and transport models (ENRESA-UPV/UPC, JNC-Golder and Nirex-Serco) apply calibration of the transport aperture/porosity and dispersivity to have correct advective behaviour. The two 1D models fit flow velocity and correlation length over the velocity field (Posiva-VTT) or groundwater residence time distribution directly (SKB-WRE).

There are two completely different concepts that can explain the transit time distribution (or residence time distribution of the examined ideal tracer). Transit time distribution may follow from the **particle trajectories that go through different fractures** and have clearly different lengths and flow velocities, i.e. from **mechanical dispersion**. This may be dominant process when the **source area is large** compared to the mean distance between fracture intersections (on the fracture planes) and mean length of the fracture traces, cf Figure 5-19a and b. The flow field has a governing influence on the residence time distribution in this case. It is noted that in this case it is also **impossible to have mixing between different trajectories** and the **residence time distribution may easily contain multiple peaks.**

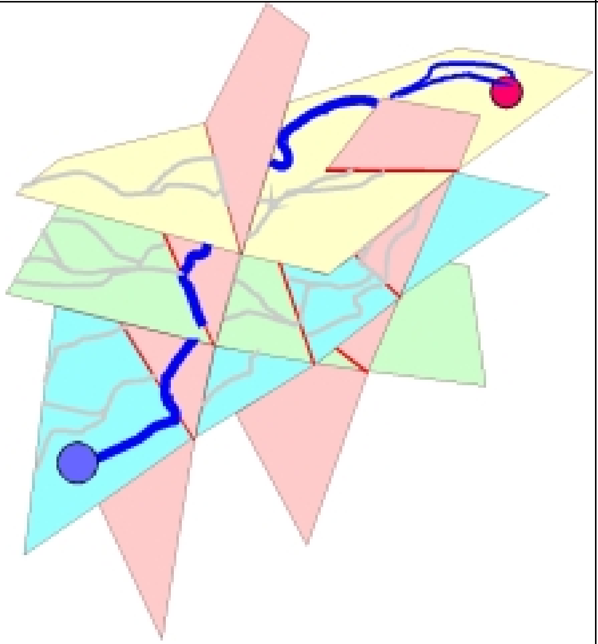
If the **source area is small** in the scale of the fracture network then **the particle trajectories tend to keep closer to each other** (in a relative sense) during the migration. In this case the flow path is nearly one-dimensional (streamtube). This case more reflects the conditions of the Phase C tracer tests, cf Figure 5-19c. Also in this case the distribution of the flow velocities and variation in the lengths of the trajectories can be described statistically using dispersion. However, the system does not usually show multiple peaks or substantial changes under small variation of the flow field. In the case of a small source area it is also **possible to have mixing across the streamtube**. This mixing originates from **molecular diffusion** that enables the tracer molecules to visit different streamlines. This leads to Taylor dispersion that averages the residence time distribution towards a normal distribution.

In order to compare the model approaches for an ideal advection situation with the purpose of obtaining the groundwater residence time distribution, **simulations of a Dirac pulse input signal** have been made for all approaches without taking diffusion or sorption into account, cf Figure 5-20. The results show that the 1D approaches – unlike the 3D SC, DFN and DFN/CN approaches – contain insignificant dispersion introduced by the flow field. It is noted that the most profound dispersion in the 3D models is introduced by Test C2.



a) Ambient natural flow conditions. Large source marked with dark blue region on the left. Active flow paths indicated by dark blue.

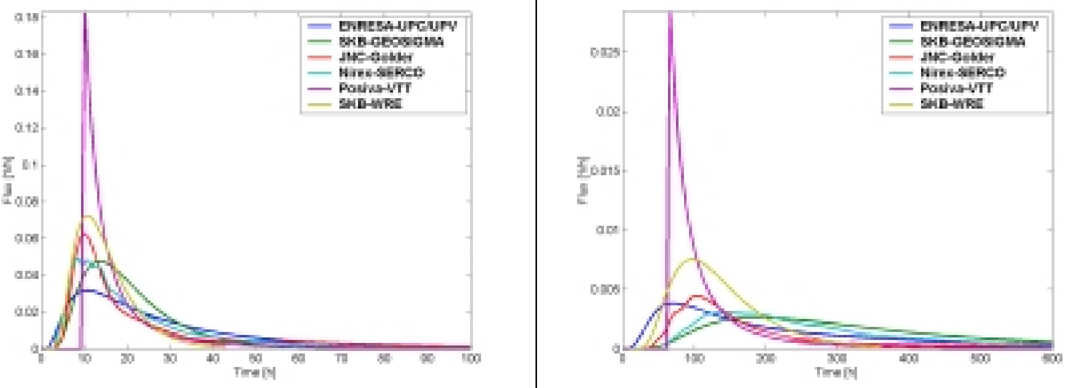
b) Sink in the model indicated by red circle. Large source area marked with dark blue region on the left. Active flow paths indicated by dark blue.



c) TRUE Block Scale Phase C conditions. Small source marked with dark blue circle and sink with red circle. Active flow path indicated by dark blue.

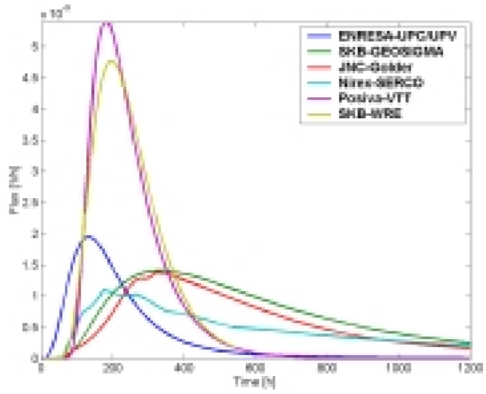
Note that FIZs are marked with red lines in the fracture network and in some cases the flow paths go along the FIZ.

Figure 5-19. *Schematic illustration of the influence of the boundary conditions and source and sink sizes on the fracture network transport.*



Tracer test C1

Tracer test C2



Tracer test C3

Figure 5-20. *Groundwater residence time distributions (no matrix diffusion/sorption) for the C1, C2 and the C3 tracer tests as provided by the different models.*

Hydrodynamic control of the retention (in terms of the parameter β, cf Equations (5-3) through (5-6)) in different models can be estimated based on the information on the groundwater transit times and retention apertures /Poteri et al, 2002/. Figure 5-21 presents β's for the different flow paths and different evaluation models. Flow path I (C1) shows a consistent grouping of most of the models showing values between 20 to 60 h/mm. It is noted, that flow path I gave breakthrough for the largest number of tracers and thereby the constraining power of the breakthrough curves is highest for this flow path. The retention parameter β should increase with increasing path length which is also clearly seen (estimated path lengths C1<C3<C2). The complexity of the flow path may have increased the spread between different models in the case of flow path II (C2). However, tracer tests C1 and C2 were performed using forced injection that may have had an impact on the parameter β. Normalising the parameter β for different flow rates and path lengths ($W=\beta/2*q/L$, cf Equation (5-3)), indicating an equivalent transport width of a uniform channel representing the physical flow path, shows values of W for the models that are 2 m to 5 m for C1 and 0.2 m to 1.5 m for C2 and C3. Generally, W is a factor of 3–5 higher for C1 than for C2 and C3. It is also noted, that test C2 showed a breakthrough only for two of the tracers over the "official" monitoring time (3300 hours).

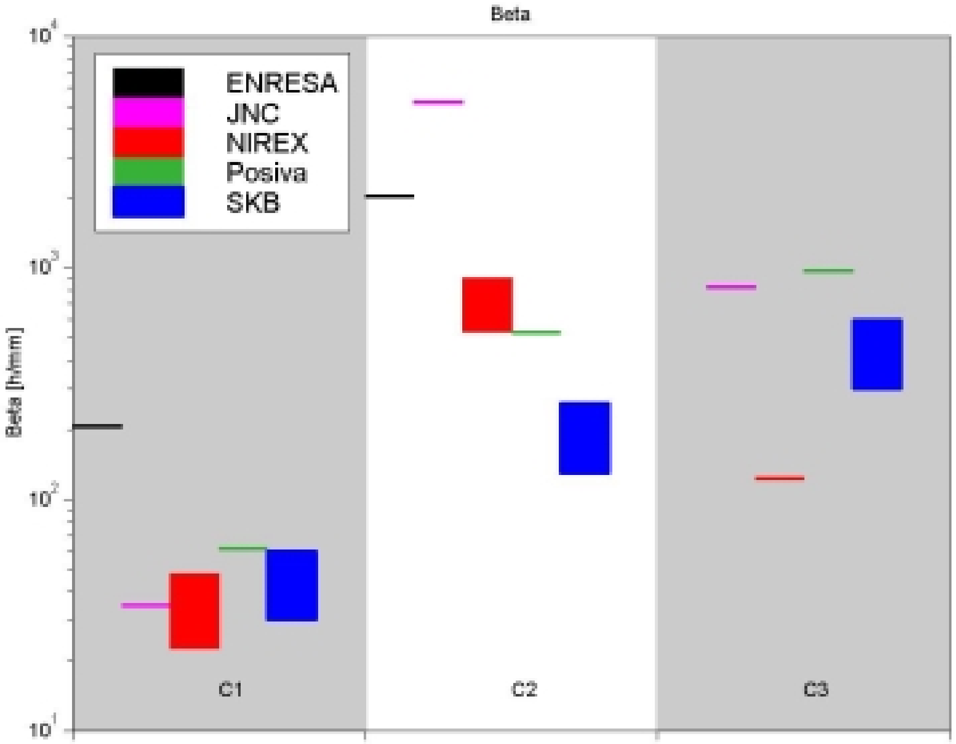


***Figure 5-21.** Evaluated parameter β that describes the average flow geometry of the flow paths of the various models and flow paths (tracer tests).*

5.6.2 Retention due to diffusion

Diffusion to the immobile pore spaces associated with the flow paths, sorption within the available immobile pore space and surface sorption on the fracture surfaces are interpreted to be the main retention processes applied in all prediction and evaluation models applied to the TRUE Block Scale experiments /Poteri et al, 2002/. The main supports for this interpretation are the residence time distributions associated with the TRUE Block Scale experiments (for both sorbing and non-sorbing tracers) which show tailing (–3/2 slope in log-log) and spreading that may be indicative of diffusive processes /Andersson et al, 2002b/. It is noted that existence of an internal boundary in the immobile pore space, or changes in diffusion properties with depth would change the slope of the tailing. A reliable estimation of the characteristic tailing indicative of diffusion processes requires a sufficiently long monitoring time. This is possible for the more strongly sorbing and long-lived tracers. However, even the appearance of the breakthrough curves of the non-sorbing species may provide indication of diffusion. The simulations show that the measured residence time distributions can be more accurately reproduced when the effects of diffusional mass transfer are invoked /Poteri et al, 2002/.

As shown in Chapter 3 there are geological evidence of a number of **immobile pore spaces** along the flow paths that could provide diffusion. Among them are the rock matrix (including the altered rim zone), fine-grained fault gouge, fault breccia and stagnant zones, cf Figure 3-4. **Molecular diffusion** is an important process that provides mass transfer between the mobile and immobile pore spaces. At this level of complexity there is no difference between the behaviour of sorbing and non-sorbing tracers in the same streamtube. During the tracer test they spend the same time in the water phase. All tracer molecules of a given tracer cocktail collected at a given time at the pumping point have spent the same transit time, or strictly speaking the same pdf (probability density function) of time in the mobile zone. The noted differences in overall residence time arise from differences in the times sorbed tracer molecules have spent on the surfaces of the mobile and immobile pore spaces.

Molecular diffusion also plays a role for the transport in the mobile pore space (fracture). In this case the tracer molecules are not retarded, since they remain at all time in the flow field. Instead the change in the residence time distribution is caused by particles in low velocity areas visiting high velocity areas, and vice versa. Diffusion in this case evens out the advective transit time distribution and attenuates the tailing of the breakthrough curve. The relative significance of this effect is very much dependent on the flow field. In the case of multiple paths, diffusional mixing is not possible as in the case of a single (“one-dimensional “) flow path, and in a case strongly dominated by advection, this process have time to influence only over a short distance.

There are immobile pore spaces, like the altered rim zone of the fracture wall rock, which have a distinctly higher porosity than the unaltered rock matrix at distance from the fracture /Byegård et al, 2001; Andersson et al, 2002a/, cf Section 3.5. However, the total volume of enhanced porosity, i.e. its **retention capacity** is, in relative terms, small. This limited capacity may be an important factor for some of the immobile pore spaces, such as for fine-grained fault gouge, altered rim zones and stagnant zones. If a given immobile pore space becomes saturated it will cease to show a mass transfer behaviour characterised by kinetically controlled diffusion. In practice this situation cannot be distinguished from other equilibrium sorption processes (such as surface sorption). An interpretation of associated breakthrough curves in this case would show enhanced surface sorption.

The immobile zones presented in Section 3.4 exhibit differences that may influence the retention properties, such as the total volume/thickness of the available pore space. It is obvious that the rock matrix (including the intact and unaltered rock away from the fractures) provides infinite capacity in practically any type of *in situ* tracer experiment. Contrary to the rock matrix, the fine-grained fault gouge is composed of small particles of rock and/or clay that have very limited capacity due to their limited thickness. It is therefore likely that for fault gouge the effects of matrix diffusion will dissipate, and that the associated retardation can be modelled as part of the equilibrium surface sorption. The latter approach is adopted by the SKB-WRE team /Cvetkovic and Cheng, 2002/. The behaviour of the tracer in the stagnant zone is assumed similar to that of the fault gouge, although the capacity may be higher. The capacity of the fault breccia (pieces and fragments) is assumed falling between that of the fault gouge and the rock matrix. Most likely, within the time frames of *in situ* tracer tests, the capacity of the fault breccia pieces does not differ much from that of an infinite medium. More importantly, in addition to variable pore space capacity, the multiple and parallel appearance of available immobile pore spaces along the tested flow paths **cause superposition of similar response characteristics** which appear in an integrated form in the *in situ* breakthrough curves. This means that it is virtually impossible to distinguish the contribution of diffusion to different pore spaces using the breakthrough data alone.

Tracer retention is governed by the **integrated (effective) retention property** along the flow paths. This integrated property is composed of the porosity and pore diffusivity of the immobile zones paired with the sorption properties of the tracer and rock, and properties of the flow field (parameter *B* in Equation (5-2)). It is not possible to back-calculate individual values of individual physical retention parameters, or at any rate, to obtain unique solutions. The interpretation of retention properties from breakthrough curves is also strongly tied to the underlying assumptions of dispersion in the advective flow field and equilibrium surface sorption. Both of these processes can produce similar characteristics in the breakthrough curves as can matrix diffusion.

Heterogeneity in the immobile zone properties may influence the interpretation of tracer retention. As an example, site-specific measurements /Byegård et al, 2001; Kelokaski et al, 2001; Andersson et al, 2002a/ indicate that the porosity of the rock matrix (altered rim zone) changes substantially close to the fracture surface, cf Figure 5-22. The porosity in the immediate vicinity of the fracture surface is much higher than the average porosity in the intact (unaltered) rock (within an order of magnitude). This zone of limited extent adjacent to the fracture surface characterised by a higher porosity will indeed influence tracer retardation over experimental time scales /Cvetkovic and Cheng, 2002/. This difference in porosity is also assumed to provide partial explanation of the differences in retention observed in the laboratory, compared to that seen *in situ*.

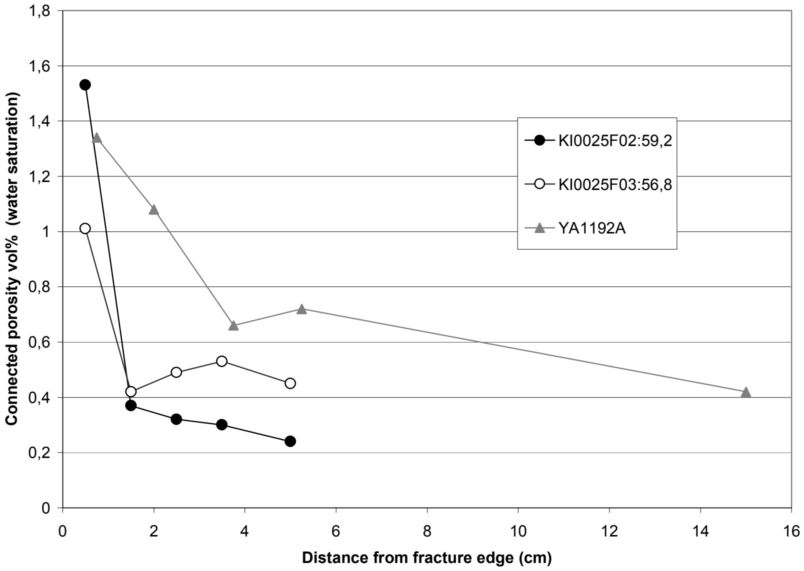


Figure 5-22. *Observed porosity values show heterogeneity. Examples of observed heterogeneity in the porosity profiles from the fracture wall into the altered wall rock matrix /Andersson et al, 2002a/. Profiles from Structure #23 established on core samples from boreholes KI0025F02 (L=59.2 m) and KI0025F03 (L=56.8 m). The sample YA1192A represents a profile from a fracture surface exposed in the tunnel /Landström et al, 2001/.*

Modelling of diffusion phenomena

Diffusion from the mobile part of the pore space to the immobile part is modelled in all model approaches as a **one-dimensional process**. This allows some freedom for the geometrical definition of the structure of the pore spaces. The conceptualisation of a typical flow path into different sub-processes of retention is presented in Figure 5-23. In a direction normal to the fracture plane the tracers experience (altered) rock matrix and possibly a thin high-porosity coating at the surface of the fracture. Stagnant pools, fault gouge and fault breccia may also be located along the fracture plane (flow path) in the lateral and normal directions to the flow path.

All five **modelling approaches** used to predict and evaluate the Phase C tracer tests **include diffusion to the immobile pore space** as a retention process /Poteri et al, 2002/. The majority of approaches account for the limited depth of the immobile zone, but the thickness of the zone varies from 0.1 mm to 1 m. One of the models (SKB-WRE) also apply a depth-dependent porosity.

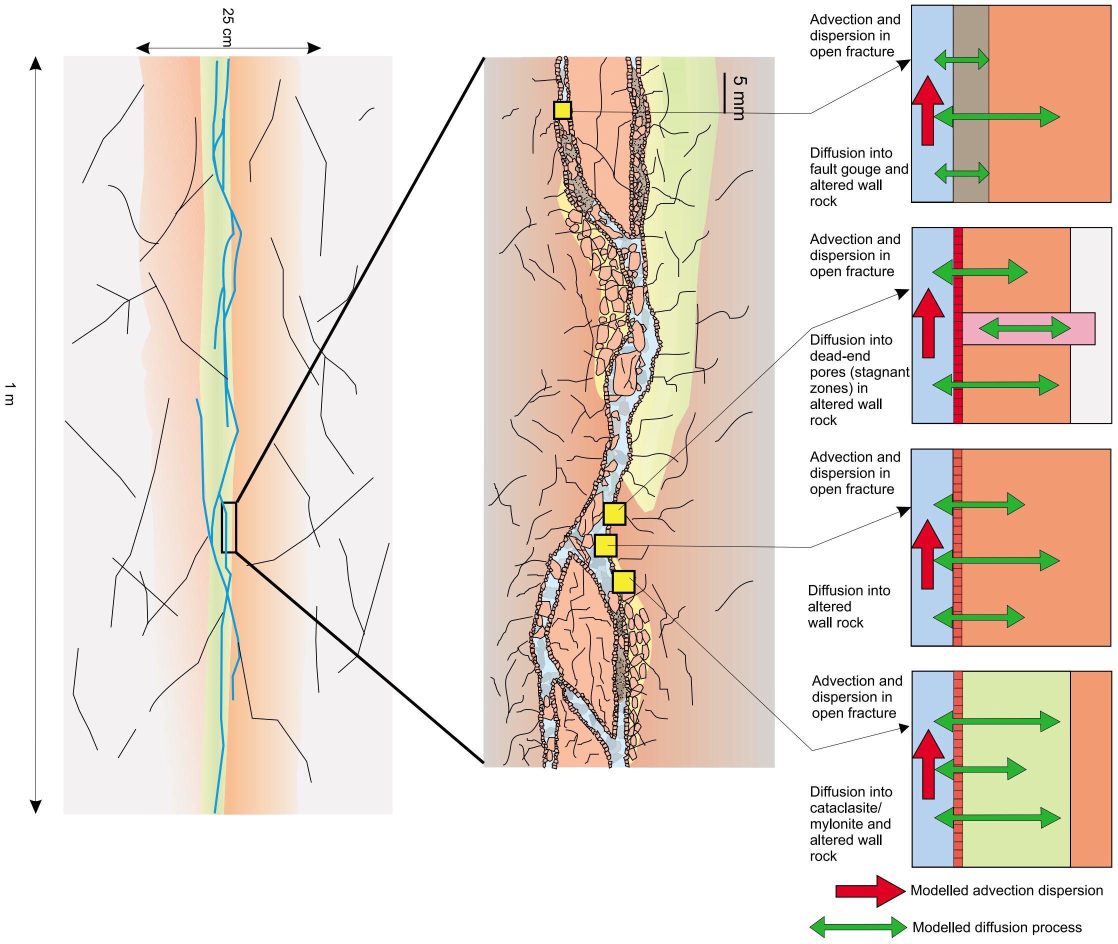


Figure 5-23. *Simplification of the pore space structure as applied in the evaluation models, cf Figure 3-4.*

For the most part the immobile zone properties are assigned in the models as effective properties that integrate the combined effects of the rock matrix, fault breccia and fault gouge. In one case (Posiva-VTT) three alternative immobile pore spaces are used /Poteri, 2002/. Overall the porosities assigned by the various teams are not that different and are also similar to the laboratory values established for the various types of immobile pore spaces /Andersson et al, 2002a/. Notably, the immobile zone diffusion properties are mainly adjusted by changing the pore diffusivity. Only in one case (SKB-WRE) non-constant pore diffusivity (function of distance along the flow path) has been considered. Despite variable attention in modelling, porosity measurements indicate enhanced porosity adjacent to fractures and heterogeneity in porosity along the flow path. Both of these aspects could be important and should be given more consideration in future modelling.

5.6.3 Effects of sorption

Transport of selected tracers and radionuclides in fractured crystalline bedrock is **reactive**. This implies that tracer particles interact with the groundwater-bedrock system by different chemical reactions along the flow paths. In transport modelling, all these various reactions, including adsorption and ion exchange, are referred to as "sorption". In the majority of situations, these reactions will retard transport of tracers, but there are also rare cases where sorbing tracer particles may migrate even faster than a non-sorbing (conservative) tracer. The latter situation may be caused by **anion exclusion** coupled with hydraulic and chemical heterogeneity.

The sorption models applied by the modelling groups to the analysis of the TRUE Block Scale Phase C experiments are based on considerably simplified representations of the real system. All models include **reversible and instantaneous equilibrium sorption** /Poteri et al, 2002/. Fixed value distribution coefficients, either volume-based K_d or surface-based K_a, are used to parameterise sorption of the different tracers used in the *in situ* experiments. These parameters only depend on the tracer, the geological material being interacted with and the composition of the groundwater /Poteri et al, 2002/. Depending on the model approach, the applied sorption values are either based on model fits to previous *in situ* experiments at Äspö HRL, and/or laboratory measurements interpreted using the K_d approach, or an estimated K_d , cf Section 3.3, or combinations thereof.

Sorption environments

Sorption will occur onto any geological material available along the flow paths. Potential sorption sites available along the paths investigated in the TRUE Block Scale tracer experiments are located in the pore spaces of the rock matrix, alteration zones around fractures, (rim zone), fault breccia pieces and fragments, fine-grained fault gouge, and on the surfaces of the fractures making up the mobile pore space, cf Figure 4-23. In conjunction with the TRUE-1 experiments /Winberg et al, 2000/ the sorption capacity of various geological materials was investigated in the laboratory /Byegård et al, 1998, 2001/. The investigations comprised experimentation on non-site-specific unaltered rock material and altered material from the mylonitic rim zone of the investigated Feature A. The investigations showed a higher sorption capacity for Äspö diorite compared to the fine-grained granite. In addition, it was found that the alteration and mylonitisation cause reduction in sorption capacity. No additional sorption experiments were conducted on geological material from the TRUE Block Scale site. Similarly, no additional experiments were conducted on the fault gouge material collected from selected intercepts with deterministic structures involved in the Phase C experiments. However, estimates of K_d for the fine-grained fault gouge were calculated on the basis of the cation exchange capacity (CEC) of selected minerals, the mineralogical composition of material of a grain size smaller than 125 μm and applicable selectivity coefficients /Andersson et al, 2002a/, cf Section 3.3. For fault gouge/fault breccia material of size fraction larger than 0.125 mm, sorption coefficients were estimated using the investigations of the altered Äspö diorite from the TRUE-1 site /Andersson et al, 2002a/. The resulting CEC-based K_d values for the finest fraction of the fault gouge showed K_d values substantially higher (a factor 20 to 60) than those based on the investigated larger size fraction from the TRUE-1 site.

Modelling of sorption phenomena

In the model approaches used to simulate the Phase C tracer tests, all sorption sub-models applied are based on linear reversible equilibrium sorption, both in the immobile pore spaces (volume-based distribution coefficient, K_d) and on the fracture surfaces (surface-based distribution coefficient, K_a). All model approaches apply K_d based sorption for the immobile pore spaces, and all but the ENRESA-UPV/UPC team has also included surface sorption.

5.7 Evaluated *in situ* retention parameters

Section 5.1 describes how retention is governed by parameter groups which accounts for the effects of the flow filed, diffusion and sorption properties. It is also noted that the evaluated *in situ* retention parameters applicable to the altered rim zone and/or fault breccia/fault gouge infillings are higher than the corresponding values related to the intact unaltered rock (MIDS data, cf /Winberg et al, 2000/ and Figure 5-24). The final evaluation models are conditioned to the measured *in situ* breakthrough of sorbing tracers. This implies that variations among the models in their advective fields or diffusion properties need to be compensated (balanced) by the selected sorption properties to produce matches to the breakthrough curves. In practice, specifying small advective dispersions, low pore diffusivities, or low porosities requires compensation with high sorption coefficients to fit the *in situ* test data, and vice versa. The following paragraphs accounts for the ranges of evaluated *in situ* retention parameters.

Porosity assigned to the immobile pore space by the various model approaches vary between 0.1 to 3%, with an extreme 50% assigned to stagnant zones by the Posiva-VTT group /Poteri et al, 2002/. **Depth-dependence** has been assigned to the rock matrix by SKB-WRE team. The **thicknesses of the immobile zones are** in the models assumed to vary between 0.1 mm to 1 m.

Assigned **pore diffusivity** for all tracers vary from about 10^{-11} m^2/s (ENRESA-UPV/UPC) to $5 \cdot 10^{-10}$ m^2/s (SKB-WRE) /Poteri et al, 2002/.

Distribution coefficients K_d applied to the least sorbing of the tracers (Na^+) varied between $2.7 \cdot 10^{-7}$ (JNC-Golder) and $2.2 \cdot 10^{-4}$ m^3/kg. Similarly, K_d values applied to one of the highly sorbing tracers (Cs^+) varied between $8.3 \cdot 10^{-5}$ (JNC-Golder) and 0.28 m^3/kg /Poteri et al, 2002/. In both cases the second, and higher, value is applicable to fine-grained fault gouge as applied by the Posiva-VTT modelling group.

The fact that the JNC-Golder team assigns the lowest K_d values and the highest pore diffusivities is an example on the balancing of retention properties to come up with an equitable net effect in the evaluation as indicated earlier in this section.

The parameter group κ provides an integration of the contribution of the evaluated retention properties to *in situ* retention, cf Equation (5-4). Figure 5-24 shows a comparison between the κ values evaluated by the different modelling groups. The figure also shows the κ value equivalent to the MIDS data set representing intact unaltered rock /Winberg et al, 2000/. A clear separation between the models as to how they apply material properties in retention is obvious from the graph. The majority of

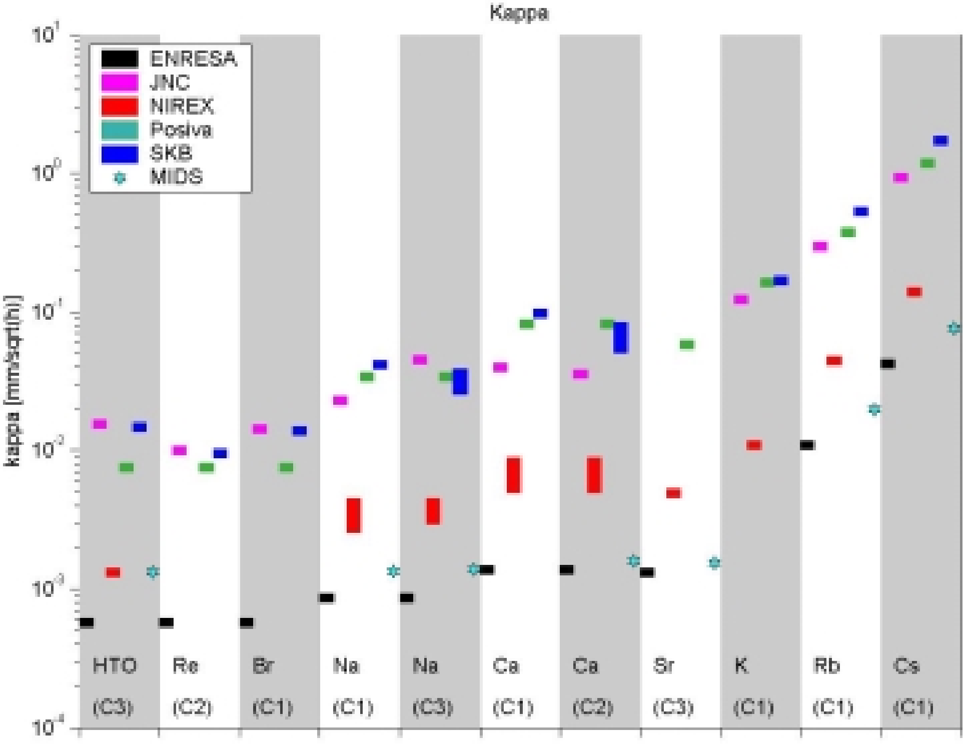


Figure 5-24. *Evaluated retention material parameter group κ (cf Equation (6-5)) for the respective evaluation models and tests (C1, C2 and C3). Compare Figure 6-2 for corresponding visualisation of input κ used in model predications.*

the models apply material properties that are clearly higher than the MIDS values. Only the stochastic continuum model (ENRESA-UPV/UPC) applies material properties that are comparable to the MIDS values. In the evaluated retention time this is compensated by the higher β values (cf Figure 5-21).

All evaluation models apply constant (**space and time invariant) distribution coefficients**. This means that the models do not address sensitivity in K_d to changing hydrochemical and geological conditions with time. In reality, the sorption processes do depend on the chemical environment. If say the pH or salinity change, a different sorption value is warranted. As an example, a successive global reduction in salinity at the TRUE-1 site from 1700 mg/l to about 1000 mg/l during the experimental phase was interpreted to have caused a 70% increase in $K_{d,}$ /Winberg et al, 2000/. It is noted that the chemical signature in the Structure #20/#13 network which was subject to the TRUE Block Scale showed a distinct signature of a mix of deep brine water and glacial water, cf Section 2.5. With time a successive influx of more fresh water was noticed in Structure #20 in the vicinity of borehole KA2563A. This influx of "alien" water is not expected to have affected the basis for interpretation of the performed experiments with sorbing tracers. However, in practise it is very difficult, if not impossible, to determine the mineralogical or hydrogeochemical variability along a transport path in time and space. Then again, from a transport modelling perspective it is not necessary to know the point to point variability, but "simply" the integrated effect along the flow path.

An attempt was made to integrate the information on parameters related to retention used by the different modelling teams /Poteri et al, 2002/. The objective being to illustrate the relative contributions to retention from the various processes/parameter groups included in the evaluation of the Phase C tracer tests. These are advection-dispersion, the hydraulic control parameter β, the material parameter group κ (diffusion/sorption) and surface sorption, cf Section 5.5 and Figure 5-25. When producing the illustration a simple weighting scheme was employed which indicates the relative importance put on a given process in a given model approach. It should be emphasised that the weights have been given subjectively by looking at the different processes included in the individual models. No direct and objective calculation method was employed to assess the relative importance of the processes. Nevertheless, the presented figure by and large indicates the relative importance of the different retention and transport processes included in the final models used to evaluate the TRUE Block Scale Phase C experiments. The different approaches are ordered vertically in descending order in terms of the overall retention.

For the most part the noted differences in mapped contribution to retention between models are explained by the differences in the modelling of the advective field. Continuum and DFN models (ENRESA, Nirex) give more variable advective transport than one-dimensional models (Posiva, SKB). The channel network model (JNC) is located somewhere in-between these two groupings. Hydrodynamic control of the retention (β) is largest in the continuum model (ENRESA) where the flow may be divided between several fractures. The hydrodynamic control in the case of one-dimensional (Posiva and SKB) and channel network models (JNC) are equitable. The diffusional coupling of the retention is adjusted by also adjusting the material properties group (κ).

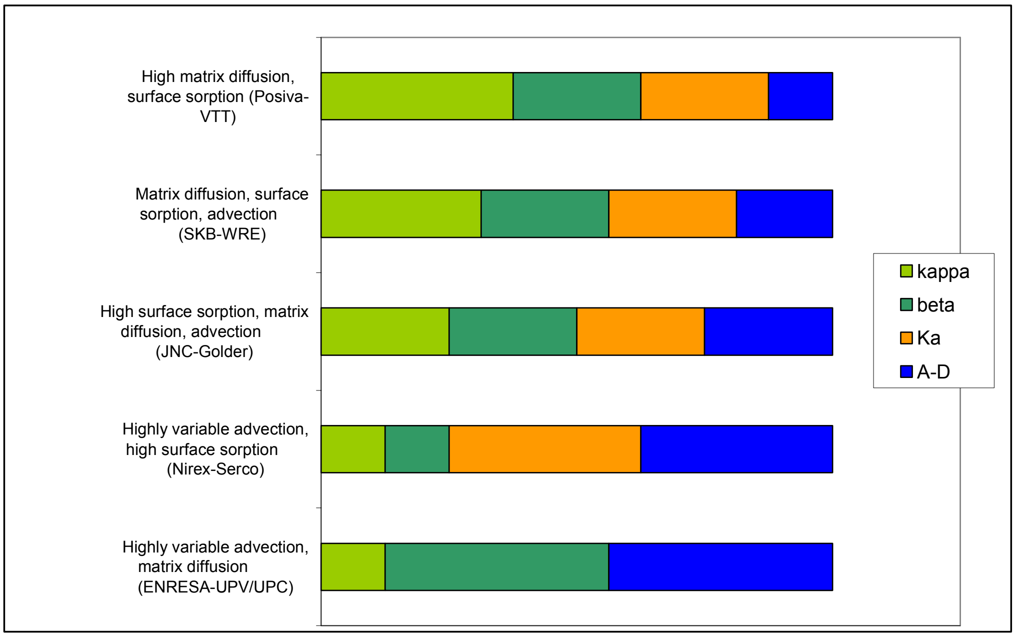


Figure 5-25. *Visualisation of subjective ranking of relative importance of retention and transport processes in models used to evaluate the TRUE Block Scale Phase C tracer tests.*

5.8 Relative importance of input data

Effect of evolving hydrostructural model

The possibility to effectively use numerical modelling in the planning of the different characterisation steps was restricted by the maturity of model and speed at which the model is constructed and updated.

In retrospect, the lack of modelling support for the planning of the tracer tests did not adversely affect the programme results. A modelling study using a DFN/CN model /Rachez and Billaux, 2002/ shows that when three selected tests from Phase B were simulated using older versions of the hydrostructural model (and associated material properties), the “fit” between measured and simulated results successively deteriorated with “relative age” of the hydrostructural model. Not even the use of the most recent calibrated material properties could improve this result at any given time.

Geological and mineralogical information

Information on site-specific pore diffusivity applicable to the immobile pore spaces is not available from the TRUE Block Scale site. However, geometry (thicknesses and extents) of the various zones are available from the PMMA analysis /Kelokaski et al, 2001/ and the core logging /Andersson et al, 2002a/. Similarly, the PMMA analysis provide data for parameterisation of porosity, including mm-sized fault breccia fragments and cm-sized fault breccia pieces, and perhaps more importantly, for the conceptualisation of a type structure. In addition conceptual and part parametric support is provided for assignment of heterogeneity in porosity in conjunction to fractures. Additional support is provided by results from a similar structure at the TRUE-1 site /Byegård et al, 1998, 2001/.

5.9 Comparison with TRUE-1 relative retention

Although the results for flow path I indicated less pronounced diffusion, cf Section 4.2.1, a good match of the breakthrough curve, particularly for the tails, required significant matrix diffusion as defined through the A-parameter /Andersson et al, 2002b/. The A-parameter incorporates hydrodynamic effects and effects of diffusion are dominant relative to that of surface sorption, cf Section 5.5. The order of retardation between the sorbing species for Path I; $Na^+ < Ca^{2+} < Ba^{2+} \approx Rb^+ < Cs^+$, is consistent with earlier tracer tests in TRUE-1 /Winberg et al, 2000/ and laboratory data /Byegård et al, 1998/. The retardation observed for Path I is larger than could be expected based on laboratory values based on unaltered matrix rock given by /Byegård et al, 1998/. Values of the A-parameter based on MIDS /Winberg et al, 2000/ laboratory data are about two orders of magnitude higher /cf Andersson et al, 2001c/. This implying an “enhanced” retardation of a factor 100 in this flow path compared to that based on laboratory results based on intact unaltered wall rock geological material presented by /Byegård et al, 1998/.

An enhanced *in situ* retardation relative to that based on laboratory data was also observed during the evaluation of the TRUE-1 experiments. In the latter case the enhanced retention including hydrodynamic effects and diffusion/sorption (in terms of $k \cdot \kappa$, cf Section 5.5) was found to be in the order of 32–50 (140 for Cs) /Winberg et al, 2000/. The enhancement observed in TRUE-1 was attributed to higher values of matrix porosity and/or diffusivity/sorption possibly caused by the presence of fault breccia/fault gouge, cf Section 1.4.2. In the case of flow path I evidence of fault gouge has been certified by findings in the cores /Andersson et al, 2002a/.

A comparison of flow path I (C1 injection) and the TRUE-1 flow paths in terms of the evaluated retention material property group κ shows a similar retention in the two flow paths /Poteri et al, 2002/. No rigorous attempts were made to incorporate the hydrodynamic effects on retention in the comparison of the two flow paths. However, tentative results in terms of the diffusion time (t_d) /Poteri et al, 2002/, support the indication of similar retention at the two sites.

5.10 Understanding transport from hydraulic data

Correlation between 1% tracer breakthrough and 1‰ drawdown was established in a semi-synthetic study using the TRUE Block Scale hydrostructural model and borehole array as a reference case /Paris, 2002; Poteri et al, 2002/. It was concluded that a good prediction of breakthrough from well test data could be expected if the distance between the observation sections and the pumped section is not large compared to the size of the fractures.

5.11 Predictive capability at different length scales

An acceptable predictive capability for the non-sorbing (conservative) tracers has been demonstrated for all the Phase C tracer tests. With regards to the sorbing tracer transport, acceptable results are obtained for the least sorbing species. The "fit" between predictions deteriorate with increasing sorption capacity and length scale. In conclusion, an "acceptable" predictive capability can only be demonstrated for the 15 m length scale (C1/C4 tests).

5.12 Summary on TRUE Block Scale retention

The *in situ* experimentation and modelling of the TRUE Block Scale Phase C experiments have achieved the following major findings:

- It is demonstrated that the applied transport modelling approaches share the same basic theoretical basis. The difference between the approaches lies in how heterogeneity is introduced and parameterised.

- The observed *in situ* retention cannot be explained by surface sorption alone.

- All modelling groups assign matrix diffusion as an important, if not dominant retention mechanism. The existence of diffusional process is also evidenced by characteristics of the measured breakthrough curves.

- Geological evidence indicates that other immobile pore spaces than the rock matrix are likely to exist along the studied TRUE Block Scale flow paths (e.g. fault gouge/fault breccia and stagnant zones).

- Porosity is significantly higher in the thin, peripheral layer of the altered fracture rim zone, and it decreases normal to the fracture to attain a background value of the intact unaltered rock several millimetres to a few centimetres away.

- Retention is governed by parameter groups (including descriptors for the flow field, immobile zone diffusion properties and sorption), cf Section 5.5. It is therefore difficult to fully discriminate between the basic retention processes and come up with unambiguous *in situ* values on retention parameters without additional constraints. Such constraints are provided by site-specific and generic laboratory data on porosity and porosity distributions provide constraints in this context, as does site-specific laboratory data on sorption and diffusivity from the TRUE-1 site. Assignment of a low sorption coefficient may be compensated with a high diffusivity providing the same net result. Notwithstanding, the results show that with slightly different assumptions, reasonable *in situ* parameter values are retained/estimated.

- Heterogeneity in retention properties of the immobile zones (along and normal to the transport paths) may have an important influence on the interpretation of *in situ* results. Possibly most important is heterogeneity normal to fracture surface (effect on kinetics, effective properties) and may provide a partial explanation of differences between predictions based on laboratory retention data and *in situ* measurements.

- The observed *in situ* retention of the TRUE Block Scale flow paths is similar to that observed in the flow paths investigated as part of the detailed scale TRUE-1 experiments.

- No additional phenomena/processes are required to explain the results of the TRUE Block Scale. The same basic model used for single structures as applied to the TRUE-1 experiments is also applicable to a network of structures. This finding is attributed to the integrating nature of matrix diffusion process. It should be pointed out that it cannot be ruled out that the configuration of the tracer tests to some extent bias this conclusion (small source area, slight injection overpressure which generally results in 1D flow paths and single peak breakthrough curves).

6 Major accomplishments

- **Useful toolkits for site characterisation**
  The TRUE Block Scale Project has confirmed the value of a number of powerful but uncomplicated characterisation techniques. Posiva flow logs identify the conducting intervals in boreholes. BIPS borehole imaging and BOREMAP core provide geologic descriptions of the conductors. Single-hole transient tests produce reliable information on hydraulic properties. Pressure monitoring during drilling and hydraulic testing indicates the connectivity along conductive features between boreholes. Additional information from long-term pressure monitoring, hydrogeochemical sampling of groundwater, and background groundwater flow, provide a basis for conceptualising the flow system in the studied rock volume. It is noted that hydrochemical data provide support for a partly compartmentalised system.

  It is also noted that geophysical methods (borehole radar and cross-hole seismics) in this particular application only played a minor role in the early phases of characterisation. One important exception is the resistivity measurement which is included in the Posiva flow log, and which further constrained the location of the conductive fracture in the borehole. Likewise, the salinity and temperature of the UCM flow meter /Andersson et al, 2002a/ were useful when inferring flow directions and in/outflow of warmer/colder and saline/fresh waters to the investigated rock block.

  It should be emphasised that the characterisation of the TRUE Block Scale rock volume has benefited from the fact that the investigated block is a) accessible from the underground, b) is relatively permeable. These two aspects combined made the hydraulic characterisation and inference relatively easy. In other situations other tool-kits may be equally effective, or better.

  At any rate it is firmly believed that the methodology employed in the TRUE Block Scale Project can be applied to block scale characterisation, whether administered from the surface or from underground openings. In the former case, a conceived scenario may be that the methodology is employed to obtain early knowledge of the area between larger fracture zones. In the latter case, the techniques are applicable for assessing potential locations for storage tunnels and/or positions for canisters.

- **Integrated network characterisation methods succeeded in providing an adequate hydrostructural descriptive model to support block scale experiments**
  Within the limitations imposed by the underground openings and possible collar positions for drilling the developed borehole array is deemed to have provided an acceptable basis for establishing the hydrostructural model of the studied rock volume. The geological, geophysical, hydrogeological and hydrochemical investigations have provided a satisfactory and mutually supportive basis for the *in situ* experimentation. This applies to hydrostructural model construction,

conceptualisation of flow paths and identification of flow paths for tests with radioactive sorbing tracers. We know from our results the intricacy of some of our identified structures. Structure #20, intercepted by all boreholes, is known to have alternate appearance at the various intercepts. Similarly, the exact nature of the interplay between Structures #13 and #21 is not known in full, but plausible hypotheses have been put forward.

- **Improved description of porosity and porosity distribution**
  The laboratory data has contributed new insight into the heterogeneous nature of the flow paths. We know more from our results about the porosity characteristics of the constituents of fault breccias. Similarly, additional support has been presented regarding the decreasing trend in porosity normal to the fracture surfaces observed already in conjunction with analysis of the TRUE-1 experiments. There is an obvious lack of site-specific TRUE Block Scale retention parameters derived from the laboratory. This applies to sorption and diffusivity data related to relevant flow paths. However, with regards to porosity characterisation the situation is much better with mutually supporting data both from water saturation and PMMA impregnation. Given the overall similarity between the TRUE-1 site and the TRUE Block Scale site, in terms of mineralogy, hydrochemistry etc, the lack of diffusivity and sorption data specifically from TRUE Block Scale material was not considered a major problem. However, given the verified existence of fine-grained fault gouge in many of the structures involved in the tracer experiments, there is an obvious lack of hard retention data on fine-grained fault gouge. This has in part been compensated by estimated sorption coefficients based on CEC, mineralogy and selectivity coefficients. However, there is a definite need for data primarily on *in situ* porosity of the fault gouge.

- **Improved conceptual microstructure models of conductive structures/fractures**
  Conceptual models for conductive fractures in fractured crystalline rock have been significantly improved through the work performed within the scope of the Fracture Characterisation and Classification (FCC) /Mazurek et al, 1997; Bossart et al, 2001/ and the TRUE programs at Äspö. Although the conceptual components are defined and geometrically conceptualised, it is yet to fully quantify some of its constituents (e.g. porosity/diffusivity of fine-grained fault gouge). Additional work is being planned to assess the latter parameters (porosity foremost) through *in situ* epoxy impregnation. An additional uncertainty which also is to be resolved is the areal distribution of the fault gouge. It is envisaged that progress on this latter issue can be achieved e.g. through genetic studies of fault (breccia) formation.

- **Simplified description of far-field from a performance assessment perspective**
  The evaluation of the results of the TRUE Block Scale *in situ* experiments so far has not required any additional phenomena/processes, relevant to the safety analysis, which were not known from previous experience from TRUE-1. Within the scope of addressing Hypothesis #2, attempts were made to assess whether fracture intersection zones could affect transport and retention. The modelling performed using the DFN/CN approach, whether in scoping mode or addressing available *in situ* results, could not show any significant effect. It is noted, however, that longer flow paths tend to show reduced mass recovery compared to shorter flow paths. This implies that tracer mass could be lost by fracture intersection zones in

hydraulic contact with an additional sink. At a smaller scale the effects of FIZs are not evident. This can be explained in two ways, either the borehole array and source-sink combinations used were insensitive to the effects of FIZs. Alternatively, the FIZs are heterogeneous in their constitution, accounting both for enhanced conductivity/transmissivity and effective barrier function provided by fault gouge infillings.

At the onset of the TRUE Programme, one of the expectations was that *in situ* retention would tend to be different when taking the step from a single fracture (detailed scale, L < 10 m) to the block scale (10–100 m). The consequence would be that some type of spatial scaling of retention parameters would be necessary when taking the step in length scale. The results from the TRUE Block Scale experiments with sorbing tracers, run over projected length scales 15–100 m, show comparable retention to what was observed at the TRUE-1 site (5 m length scale) /Poteri et al, 2002/. This indication, although of limited statistical significance, may indicate that complicated spatial scaling or parameters when taking limited steps in length scale is not necessary. Analysis of the step in spatial scale from laboratory (< 0.5 m) to detailed and block scales is partly obscured by the fact that the majority of laboratory data are derived form experiments on intact unaltered geological material.

It should be pointed out that the step in spatial scale was not associated with a step in temporal scale. Evaluation of the effects of taking a step in time scale from experimental (1–2 years) to performance assessment time scale (10^4–10^5 years) is not easy to assess. It is expected that the microstructural model adopted and its parameterisation may have a strong impact on long-term performance.

- **Identification of retention data needs for repository site characterisation**
  Over the practical time frames of *in situ* experimentation, the retentive capacity provided by the near proximity rock adjacent to conductive fractures/flow paths will be involved in the retention of tracers. This combined with the defined parameter groups accounting for the individual retention processes, calls for improved laboratory quantification of diffusivity, porosity and sorption applicable to experimental time scales. It should however be emphasised that a laboratory programme will never account for the exact mix of properties which solutes will experience along a given physical flow path. Effectively we are only in a position to assess the situation at the source and at the sink. Exhaustive laboratory tests and statistics can in principle resolve this problem of uncertainty, but there is no guarantee to fully understand the particular flow path. In essence, we only know the integrated response of a given flow path and our job is, to the best of our ability, to narrow down and constrain the *in situ* parameter estimates.

  In the perspective of site characterisation for a geological repository, and subsequent performance assessment, the situation is different. Over the time span of a geological repository the retentive capacity of the close proximity rock (altered rim zones, fault breccia/fault gouge) will be consumed relatively quickly. This implies that the retentive capacity of the intervening rock blocks can be viewed as essentially infinite. However, this assumption is very much dependent on the extent of the connected porosity beyond the altered rim zone. At present, firm proof of infinite capacity is not available. Hydrothermal alteration haloes centred on conductive fractures, which can be regarded as natural analogues in this context, are by no means infinite, but rather have finite extents. On the other hand the extent/distribution of alteration haloes seem to be uniform. From a performance assessment perspective there is a need to show what capacity (extent of connected porosity) that is required to safeguard release to the biosphere of non-harmful activities of radionuclides. The altered rim zone and fault breccia/fault gouge of fractures making up potential pathways for particles released from a geological repository provide an extra, although limited, contribution to the safety margins of a geological repository. Through their elevated contents of clayey materials they provide ample opportunity for slow reversible sorption, or even irreversible fixation of certain radionuclides.

Given the experience of this project, a repository site characterisation effort should first emphasise the descriptions of drill cores and borehole image logs to identify the geologic features that potentially could have significant retentive capacity. This first effort would also quantify the intensity of fractures and structures that exhibit these characteristics. A second level of effort would include laboratory measurements to quantify the properties that affect retention and to directly measure retention properties, such as K_d. In the case recovery of geological materials from drill cores is found difficult, experimental data could be imported from available underground facilities (RCFs, URLs or mines) in relevant geological environments.

- **Inherent limitations in site characterisation with regards to collection of data relevant to PA**
  The methodology employed in TRUE Block Scale does not provide a direct means to assess the flow-field controlled contribution to retention through parameters like β (or 2WL/q), cf Section 5.5, from site characterisation data alone. The parameter 2WL/q can however be estimated one the basis of geometrical inferences paired with flow data, the latter either from borehole flow data (ambient flow rate from tracer dilution tests) or from modelling. Alternatively the parameter β can be estimated using model simulation.

- **Relaxation of conservative assumptions**
  The improved conceptualisation and parameterisation of fracture rim zones and infillings can add additional margin to the safety case. This applies especially to those radionuclides, which are expected to be fixated permanently by clay minerals associated with the altered rim zones and fracture infilling materials.

7 Ongoing and planned future research

The TRUE Project has ongoing continuation projects which include work performed at both the TRUE-1 and TRUE Block Scale sites.

Continued work related to the TRUE-1 site is associated with the uncertainties remaining at the termination of the TRUE-1 project which were discussed further at a subsequent international seminar /SKB, 2001/. The ongoing and planned work is included in the **TRUE-1 Continuation Project** and is made up of the following components;

- Complementary *in situ* experiments with the objective of shedding light on remaining **conceptual uncertainties** such as reasons for observed double peak and three-dimensional flow effects on transport. *In situ* tests include cross-hole hydraulic interference tests, tracer dilution tests and cross-hole tracer tests performed early 2002 /Andersson et al, 2002c/.

- Development and test of methodology to infer **aperture of conductive fractures** from radon concentration in groundwater samples collected from discrete test sections in the TRUE-1 array paired with radon flux measurements on geological material. Time perspective: 2001–2003.

- **Characterisation of fault rock zones** of variable size using e.g. resin injection and subsequent excavation. Special emphasis on the *in situ* porosity of fine-grained fault gouge. Time perspective: 2002–2004.

- Laboratory determination of **sorption characteristics of** geological materials from the **altered rim zone and fault gouge**. Materials collected from the TRUE Block Scale site and from other sites, possibly from the fault rock zones indicated above. Time perspective: 2003–2004.

- The ultimate step in terminating experimental activities at the TRUE-1 site is **impregnation of the tested feature** near an injection section **using an epoxy resin** or an equivalent agent. Careful excavation and analysis will follow where the **geometry of the pore space** is assessed as well as the **fixation of the long-lived radioactive tracers** used (^{137}Cs). Time perspective: 2005–2006.

Complementary to the above planned *in situ* porosity determination of fault gouge materials is the **Long-Term Diffusion Experiment** (LTDE) /Byegård et al, 1999/ that is primarily focused on the properties of the intact unaltered rock. The experiment will be performed in a telescoped borehole centred on the altered and unaltered bedrock in conjunction with a conductive fracture located some 10 m from the wall of the access tunnel. Groundwater traced with radioactive tracers, some of them sorbing, will be circulated in test sections contacted with the natural fracture surface and the intact rock for a period of 3–4 years. Subsequently the rock mass involved will be overcored and sampled for tracer concentration. Inferred *in situ* diffusivity parameters will be compared with corresponding results obtained in the laboratory on core samples. The experiment is expected to a) provide demonstration of *in situ* matrix diffusion, b) shed light on effects of mechanical effects related to porosity/diffusivity determination on drill cores, c) provide additional understanding related to sorption and sorption environments in the vicinity of a fracture rim zone of a conductive fracture.

The “official” termination of the TRUE Block Scale *in situ* experiments (Phase C) was in November 2000. At that time most of the short-lived radioactive sorbing tracers had either showed breakthrough or decayed completely. However, some of the long-lived tracers administered in the longer flow paths (C2 and C3) had not showed breakthrough. Sampling was therefore continued on a low-intensive level and is still in progress in August 2002.

One of the objectives with a **TRUE Block Scale Continuation Project** is to analyse the tails of the breakthroughs and also to analyse additional breakthroughs observed in the prolonged sampling. In addition, complementary modelling based on the results of the Phase C evaluation modelling and the new breakthrough data is expected to provide support and pave the way for new hypotheses to be tested in complementary *in situ* tracer tests. Another aspect that will be pursued is assessment of comparative performance measures for *in situ* retention relevant to performance assessment. This includes assessment of 2WL/q and β measures and revisit of inclusion/attribution of heterogeneity in retention parameters, or alternatively assignment of effective retention parameters.

The overruling objectives of the TRUE-1 Continuation and TRUE Block Scale Continuation projects are to;

- Demonstrate and validate a process for defining the critical geologic elements for flow and transport/retention and their transport properties.

- Define, at different scales, the pore space (responsible for) necessary to explain transport, diffusion, sorption and loss of tracer.

- Integrate experimental results from the laboratory, detailed scale and block scale to obtain a consistent and adequate description of transport to serve as a basis for modelling transport from canister to biosphere.

All the above stated objectives serve to further improve understanding of transport and retention at different length scales. In this context optimal usage of resources and infrastructure at the two experimental sites will be employed. It is expected that the conceptual understanding gained combined with evaluated transport parameters will serve to better constrain PA models. In addition, it is also expected that the planned work will help focus site characterisation programs to collect relevant information important for performance assessment.

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