

# Evaluation of modelling of the TRUE-1 radially converging tests with sorbing tracers

## The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes

### Tasks 4E and 4F

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May 2001

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*Keywords:* Äspö, Crystalline rock, sorbing tracer tests, groundwater flow, transport of solutes, modelling

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

## Abstract

The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes is a forum for the international organisations supporting the Äspö HRL Project. The purpose of the Task Force is to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock. Task 4 of the Äspö Modelling Task Force consists of modelling exercises in support of the TRUE-1 tracer tests. In this report, the modelling work performed within Tasks 4E and 4F is evaluated, which comprised predictive modelling of the tracer tests (STT-1, STT-1b and STT-2) performed within the TRUE-1 project using sorbing and non-sorbing tracers. The tests were made between packed off boreholes penetrating a water-conducting geological feature with a simple structure (Feature A).

Nine modelling teams representing eight organisations have performed predictive modelling of the tracer tests using different modelling approaches and models. The modelling groups were initially given data from the site characterisation, data from preliminary tracer tests performed with non-sorbing tracers and data on the experimental set-up of the sorbing tracer tests. Based on this information, model predictions were made of drawdown, tracer mass recovery and tracer breakthrough. For the predictions of the STT-1b and STT-2 tests results from previous tracer tests with sorbing tracer were also available.

The predictions of the sorbing tracer breakthrough in the initial tracer test (STT-1) generally underestimated the breakthrough time, suggesting the need to include additional processes and evaluate the application of the laboratory data. As a result of model calibration and modification the predictions were considerably improved for the latter tracer tests (STT-1b and STT-2).

Task 4E and 4F has proved to be very valuable in increasing the understanding of non-sorbing tracer transport in fractured rock. There is a general consensus on the major processes responsible for transport and retardation and also how these processes can be described in a mathematical model. However, there are still a number unresolved questions concerning the application of laboratory data to tracer tests, the extrapolation of tracer tests to other distances and time scales and the application of results to other sites.

## Executive Summary

The Äspö Hard Rock Laboratory (HRL) is an underground research facility situated on the east coast of Sweden operated by the Swedish Nuclear Fuel and Waste Management Company (SKB). The Äspö HRL provides opportunities to perform studies of behaviour and properties of the natural geological barriers, investigate interactions between engineered barriers and the host rock, and perform development and demonstration of technology for deep repository systems.

Within the Äspö Hard Rock Laboratory project a programme called Tracer Retention Understanding Experiments (TRUE) has been defined for tracer tests at different experimental scales. The overall objective of the TRUE programme is to increase the understanding of the processes which govern retention of radionuclides transported in crystalline rock, and to increase the credibility in the computer models for radionuclide transport which will be used in the licensing of a repository. Within the first stage, TRUE-1, a series of tracer experiments have been performed in a single feature using both non-sorbing and sorbing tracers.

The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes was initiated by SKB in 1992 as a forum for the organisations supporting the Äspö HRL Project. The purpose of the Task Force is to interact in the area of conceptual and numerical modelling of groundwater flow and solute transport in fractured rock. In particular, the Task Force proposes, reviews, evaluates and contributes to such work in the HRL Project.

Task 4 of the Äspö Modelling Task Force consists of modelling exercises in support of the TRUE-1 tracer tests. In this report, the modelling work performed within Tasks 4E and 4F is evaluated. These tasks comprised predictive modelling of the tracer tests performed within the TRUE-1 project using sorbing and non-sorbing tracers. These tests were performed between packed off boreholes penetrating a water-conducting geological feature (Feature A). A total of nine modelling teams representing eight organisations have performed predictive modelling using different modelling approaches and models.

The focus of Task 4E and 4F has been on the transport processes especially those of importance for sorbing tracers. The modelling groups were initially given data from the site characterisation, data from preliminary tracer tests with non-sorbing tracers and data on the experimental set-up of the tracer test. Based on this information, model predictions were made of drawdown, tracer mass recovery and tracer breakthrough. After the predictions were delivered to the Task Force secretariat, the experimental results were revealed to the modelling teams.

The modelling groups have basically retained the model geometry and structural model used in the predictions of the non-sorbing tracer experiments in Task 4C and 4D. The majority of groups have treated Feature A as an isolated single feature, with some

exceptions. In some cases also other features and background fractures have been included.

The predictions of the sorbing tracer breakthrough in the initial tracer test (STT-1) generally underestimated the breakthrough time. It was apparent that the active processes were more complex than initially anticipated and that the application of laboratory data was not straightforward. As a result of model calibration and modification the predictions were considerably improved for the latter tracer tests (STT-1b and STT-2). During the course of the task, the models also became more similar, concerning the processes that were considered. For the predictions of STT-2 matrix sorption and diffusion was considered by all the models, whereas only half of the modelling groups used matrix diffusion and sorption in their predictions for STT-1. However, there were still substantial differences between the different models used for the prediction of STT-2.

An important part in the Task 4E and 4F work was the evaluation done after the results of the experiment were revealed. The modelling groups have put a lot of effort in the evaluation, calibrating model parameters, modifying and adapting models and testing alternative approaches. This has proved to be a successful strategy for evaluating the importance of different transport and retardation processes. The interaction with the TRUE project has also proved to be very valuable, where discussions between modellers and experimentalists have provided additional information about geological and geochemical conditions at the site.

The tasks have proved to be very valuable in increasing the understanding of non-sorbing tracer transport in fractured rock. There is a general consensus on the major processes responsible for transport and retardation and also how these processes can be described in a mathematical model. However, there are still a number unresolved questions concerning the application of laboratory data to tracer tests, the extrapolation of tracer tests to other distances and time scales and the application of results to other sites.

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# 1 Introduction

Disposal of spent nuclear fuel in deep rock is based on the principal of multiple barriers: engineered barriers such as the canister and the backfilling material, and natural barriers such as the bedrock itself. The deep bedrock constitutes a barrier by providing a mechanically, geologically and chemically stable environment in combination with low water fluxes. Furthermore, many radionuclides interact with the mineral surfaces of the rock and are significantly delayed in their transport through the rock. This process will significantly reduce the release to the biosphere for radionuclides with a radioactive half-life considerably less than their travel time in the geosphere.

The importance of the low groundwater flow and the radionuclide retention implies that a considerable knowledge is required concerning the groundwater movement and solute transport. In safety assessments these processes need to be evaluated in large volumes of rock over long periods of time. Consequently, modelling of groundwater flow and solute transport is an important issue in nuclear waste management research programmes.

The water flow in crystalline rock occurs mainly along discrete water conducting features. Only a part of the visible fractures carries any flowing water and only a few of these fractures are responsible for the largest of the observed flow rates. There is also evidence that the flow is located to limited pathways within the fractures (Abelin et al., 1985, 1990; Bourke, 1987; Moreno and Neretnieks, 1993). These are usually referred to as channels. The actual nature of the flow paths is important for the radionuclide transport for several reasons. Firstly, it determines the size of the contact area between the flowing water and the rock, a parameter that is crucial when estimating the extent of radionuclide sorption and retardation. Secondly, how well and how frequently the flow paths are connected is of importance for the residence time distribution and thereby for the dispersion of radionuclides.

Tracer tests are one method commonly used to study the nature of the flow paths in geological media. With tracer tests various transport properties can be investigated, for example residence time distributions, flow porosity and dispersion. The results of tracer tests are also used for qualitative and quantitative evaluation of various transport processes. Comparisons with model results can provide valuable information on the capabilities of models to adequately describe the hydrology and solute transport.

## *Äspö HRL*

The Äspö Hard Rock Laboratory (HRL) is an underground research facility situated on the east coast of Sweden in the vicinity of the Oskarshamn nuclear power plant and is operated by the Swedish Nuclear Fuel and Waste Management Company (SKB). The Äspö HRL provides opportunities to perform studies of behaviour and properties of the natural geological barriers, investigate interactions between engineered barriers and the host rock, and perform development and demonstration of technology for deep repository systems.

### *The TRUE programme*

In 1994 the TRUE programme (Tracer Retention Understanding Experiments) was defined (Bäckblom and Olsson, 1994). The overall objectives are to increase the understanding of the processes that govern retention of radionuclides in crystalline rock and to increase the confidence in the computer models for radionuclide transport that will be used in the licensing of a repository. Different model concepts are evaluated with regard to realistic description of the rock, possibility of acquiring data from site characterisation, usefulness and feasibility. Within the TRUE programme a number of experiments are performed in stages at different scales and with successively increasing complexity.

The first stage (TRUE-1), completed in 2000, had the objectives to conceptualise and parametrise an experimental site using both non-sorbing and sorbing tracers in a simple test geometry, and to improve methodologies for tracer tests on a detailed scale (Winberg et al., 2000). Additional experiments performed within this stage of TRUE concerns the injection of resin in fractures for obtaining fracture aperture distributions, and testing sampling and analysis technologies for evaluating matrix diffusion. The work performed within TRUE-1 was to a large extent a learning exercise contributing data and experiences for the more elaborate tracer tests performed within the TRUE project, e.g. the TRUE Block Scale Project.

### *Äspö Task Force*

The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes was initiated by SKB in 1992 as a forum for international co-operation within the Äspö Hard Rock Laboratory. Each organisation supporting the Äspö HRL is invited to form or appoint a team performing modelling of the HRL experiments. The work within the group is being performed on well-defined and focussed modelling tasks in the area of conceptual understanding and mathematical modelling of groundwater flow and solute transport. The modelling efforts performed in the Task Force work provides information on how different model concepts can be applied in fractured rock and in particular for identification of important parameters needed to perform predictive modelling of radionuclide transport.

The Modelling Task 4 consist of several modelling exercises in support of the TRUE-1 tracer tests including predictive modelling where the experimental results are not available beforehand. Task 4A consisted of modelling in support of the development of the descriptive structural model of the test site. The scope of Task 4B was to perform modelling in support of the experimental design. Tasks 4C and 4D were defined to perform predictive modelling of non-sorbing tracer tests at the TRUE-1 site, including a comparison of model outputs with experimental results. The modelling work performed in Tasks 4C and 4D is evaluated in Elert (1999). All these tasks are to a great extent preparatory steps for Tasks 4E and 4F that comprise predictive modelling of tracer tests performed with collection of sorbing, slightly sorbing and non-sorbing tracers.

The present report gives an evaluation of the predictive modelling of the radially converging tracer tests performed within TRUE-1 using sorbing tracers. These tests were made between packed off boreholes penetrating a water-conducting geological feature with a simple structure.

A total of nine modelling teams representing eight organisations have performed predictive modelling using different modelling approaches and models. The modelling groups were asked to make model predictions based on data from the site characterisation, data on the experimental set-up of the tracer experiment and results from preliminary design tests (PDT) performed with non-sorbing tracers. After the predictions were delivered to the secretariat, the experimental results were revealed. In addition the modelling groups were asked to fill in a questionnaire concerning: issues of special interest, model and data base, calibration and sensitivity analysis performed, lessons learned and issues resolved. The purpose of the questionnaire was to obtain a rapid feedback from the modelling teams and to aid the evaluation process. The results of the experiments, the predictions and the evaluations are compiled in proceedings of the Äspö Task Force meetings (Ström, 1998) and (Morosino, 1999a, 1999b and 2000). The work performed by the modelling groups is also reported in International Cooperation Reports (ICR-reports), see Table 1-1.

**Table 1-1 Organisations and modelling teams participating in Tasks 4E and 4F**

<b>Organisation</b>	<b>Modelling team</b>	<b>Representative</b>	<b>Task 4E</b>	<b>Task 4F</b>	<b>Reference</b>
ANDRA	CEA-DMT	E Mouche	X	X	
BMWi	BGR	L Liedtke	X	X	ICR 99-03
CRIEPI	CRIEPI	Y Tanaka	X	X	ICR in prep.
DOE	SANDIA	S McKenna		X	
JNC	Golder Associates	W Dershowitz	X	X	ICR 01-02.
NAGRA	PSI	A Jakob	X	X	ICR in prep.
POSIVA	VTT Energy	A Poteri	X	X	ICR 01-01.
SKB	KTH-ChE	L Moreno	X	X	ICR 01-03
SKB	KTH-TRUE	J-O Selroos	X	X	ICR 00-01

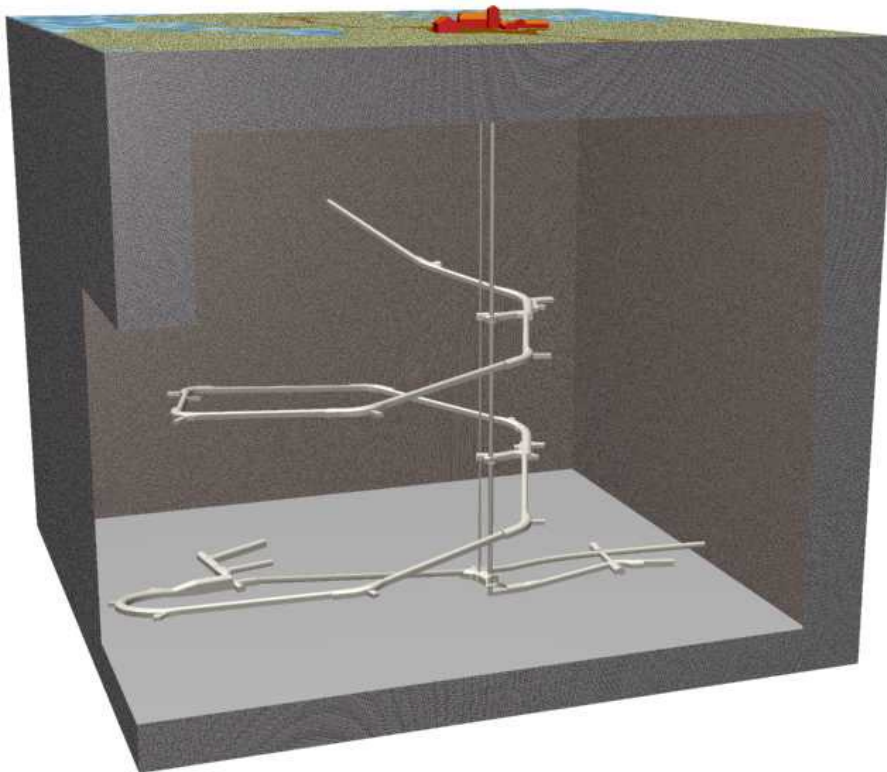
This evaluation report focuses on the lessons learned from the modelling work in terms of process understanding and model capability, rather than on how the individual modelling groups or models achieve in the predictions. In Chapter 2, the purpose and set up of the experiments subject to modelling are given. Chapter 3 presents the various modelling approaches used and in Chapter 4 a comparison between the results of the experiments and the predictive modelling is presented. Chapter 5 contains a discussion of the predictive modelling, lessons learned and remaining unresolved issues. Finally, in Chapter 6 the main conclusions of the Modelling Task 4E and 4F are given.

## 2 Purpose and set up of experiments

### 2.1 Description of settings

#### *Äspö HRL Site*

The Äspö Hard Rock Laboratory is situated on the east coast of Sweden in the vicinity of the Oskarshamn nuclear power plant. The layout of the Äspö HRL is shown in Figure 2-1. The tunnel starts at the Simpevarp peninsula and extends northward towards the southern part of the island of Äspö where the tunnel continues in a spiral down to a depth of 450 meters. The total length of the tunnel is approximately 3600 meters.



*Figure 2-1 General layout of the Äspö HRL.*

#### *Äspö tunnel and TRUE block*

The experimental site for the TRUE-1 tracer experiments, the TRUE-1 block, is a well characterised rock block of approximately 50 m scale at the northern end of the Äspö HRL at a depth of about 400 meters. A detailed characterisation programme has been performed on the site including five cored boreholes (KA3005A and KXTT1-KXTT4).

The characterisation included analysis of pressure response during drilling, core logging, geological mapping, borehole radar, mineralogical analyses, detailed flow logging, selective flow and pressure build-up tests, installation of multiple packer systems, multiple hole interference tests, hydrogeochemistry, preliminary tracer tests and tracer dilution tests. Based on the resulting database a structural model has been built (Winberg, 1996), see Figure 2-2. Three minor fracture zones (NNW-4, NW-2 and NW-3) have been identified and are interpreted as boundaries of the TRUE-1 block. In addition a structurally less well-defined zone (NW-2') was identified.

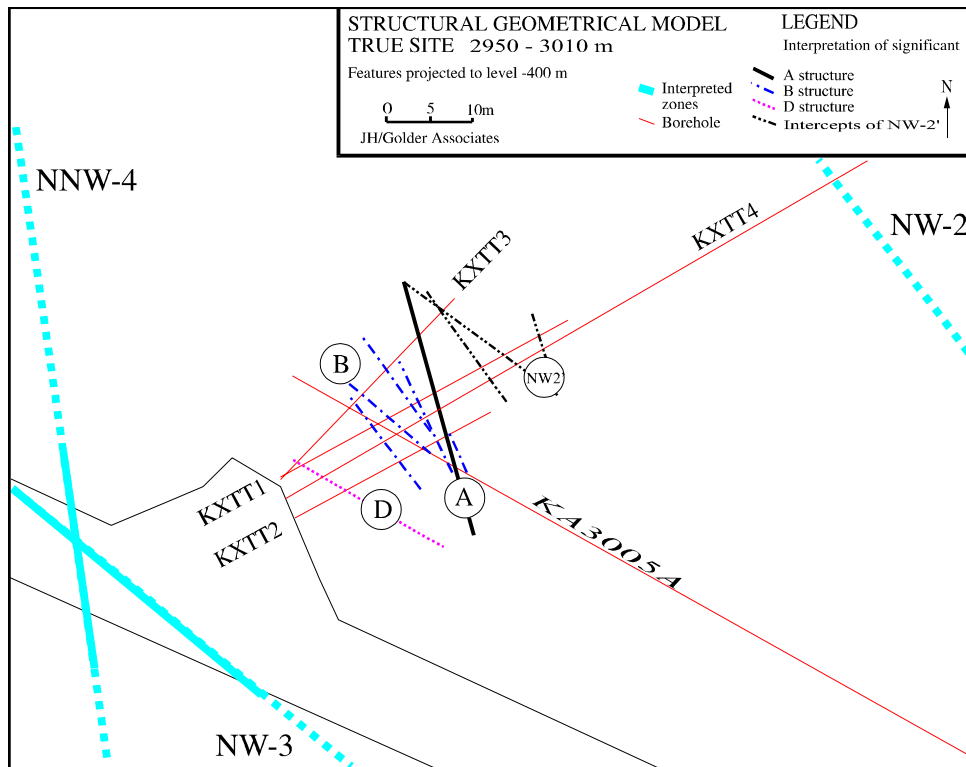


Figure 2-2 Structural and geometrical model of TRUE site. Horizontal section at  $Z=-400$  m showing bounding minor fracture zones and features identified in the TRUE-1 Block.

Four minor features (Features A, B, C and D) were identified in the borehole array. Feature A is a steeply dipping NW trending structure characterised as a reactivated mylonitic structure. Features B and D are structurally more complex, consisting of a number of different planar fractures with a wide spread in orientations making NW trending features intersecting Feature A south of the borehole array. Feature C is interpreted as a single gently dipping fracture.

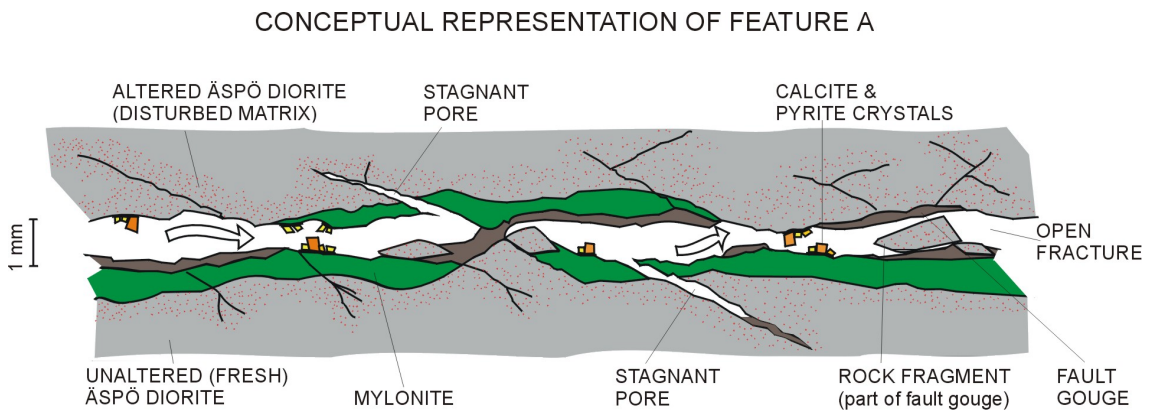
### Feature A

In the update of the structural model of the TRUE-1 block a more detailed description of Feature A is given (Winberg et al., 1998). The updated model has included the outcome of work performed as a part of the Fracture Classification and Characterisation project

(FCC) (Bossart et al., in prep) and the results of the tracer test programme (RC-1-RC-3, DP-1-DP-6, STT-1, STT-1b, STT-2).

Results of performed cross-hole interference data show that the response in Feature B and other sections not associated with Feature A is very low in within area of Feature A covered by the boreholes. This reflects the relative hydraulic isolation of Feature A. Results of the tracer tests show that Feature A is connected over the entire area covered by the borehole array. The flow path KXTT4 R3 to KXTT3 R2 shows an unnaturally high dispersivity, which could be an indication of two flowpaths belonging to Feature A intercepting section KXTT4 R3. The detailed flow logs and the BIPS (Borehole Image Processing System) image show an open fracture subparallel to Feature A in section KXTT4 R3. The fracture may possibly be regarded as a part of Feature A. Pressure response during pumping tests also indicates that Feature A is divided up in fractures (splays) towards the tunnel.

Figure 2-3 shows the schematic conceptual representation of Feature A presented by the TRUE-1 project (Winberg et al., 2000). The feature essentially follows the mylonite, but can in part be in contact with altered Äspö diorite. The main fracture minerals in Feature A are calcite, fluorite, quartz, k-feldspar and pyrite. SEM/EDS analyses show the presence of clay minerals as an outer rim of the fracture mineral coating. This has been taken as an indication that gouge material may be present in Feature A. Gouge material has been found in similar features, but has not been isolated in the core drillings performed in Feature A.



FRACTURE APERTURE TO SCALE. OTHER GEOLOGICAL UNITS NOT TO SCALE

*Figure 2-3 Schematic conceptual representation of Feature A. Note that fracture aperture is not to scale.*

An alternative conceptual model of the TRUE-1 block based on the results of the Fracture Characterization and Classification Project (FCC) is documented in Mazurek et al. (1996, 2001). In the FCC project, water-conducting features at Äspö were investigated on a wide range of scales from millimetres to kilometres. Among the main objectives were the geometric understanding of the present-day fracture network, its evolution over geological time and the characterisation of the recurrent events of hydrothermal water/rock interaction. One of the results of these investigations was the geological conceptualisation of fracture patterns and the definition of various rock



domains that may interact with migrating tracers in field experiments of short duration or in the course of long-term natural processes.

In the alternative model the TRUE-1 volume including Feature A show a highly complex network of fractures, cracks and fissures often bounded on one side by a high porous zone accessible for diffusion addressed as fault gouge material. According to this model Feature A is unlikely to be a single discrete structure, but more likely a cluster of shorter interconnected fractures that concentrate along the mylonitic precursor.

### *Preliminary design tests*

Prior and during the Sorbing Tracer Tests (STT) Preliminary Design Tests (PDT) were performed in Feature A to optimise the test configuration for tests with radioactive sorbing tracers. Four preliminary design tests have been performed (PDT-1 – PDT-4), see Table 2-1. The tracer solution used in PDT-1 and PDT-2 contained only non-sorbing tracers, the fluorescent dyes Uranine and Amino G. The tracer solution injected in the PDT-3 experiment contained both non-sorbing and weakly sorbing tracers (Uranine, HTO,  $^{82}\text{Br}$  and  $^{24}\text{Na}$ ). The purpose of including the weakly sorbing tracer  $^{24}\text{Na}$  was to give the experimental team a first indication of the sorptive properties of Feature A (Andersson et al., 1998a). However, this data was not provided to the modellers.

**Table 2-1 Summary of tracer tests performed within Tasks 4E and 4F. In all the cases pumping was performed in section KXTT3 R2.**

	Preliminary Design Tests				Sorbing Tracer Tests		
	PDT-1	PDT-2	PDT-3	PDT-4	STT-1	STT-1b	STT-2
<b>Injection section</b>	KXTT1 R2 KXTT4 R3	KXTT1 R2 KXTT4 R3	KXTT4 R3	KXTT1 R2	KXTT4 R3	KXTT1 R2	KXTT4 R3
<b>Pumping rate</b>	0.1 l/min	0.2 l/min	0.4 l/min	0.4 l/min	0.4 l/min	0.4 l/min	0.2 l/min
<b>Sorption of used tracers</b>	None	None	None Weak	None	None Weak Moderate	None Weak Moderate	None Weak Moderate

The objectives of PDT-1 were to find the lowest possible flow rate with maintained high recovery and to optimise injection and sampling procedures. The PDT-1 test was conducted as a radially converging test with injection in two sections, KXTT1 R2 and KXTT4 R3 using a pumping rate of 0.1 l/min in KXTT3 R2. The test showed a relatively low mass recovery for both paths and consequently the pumping rate was increased in PDT-2.

The objective of PDT-2 was to check that boundary conditions were unchanged compared with previously performed dilution tests. The PDT-2 test was conducted as a radially converging tracer test with injection in the same two sections as in the PDT-1 experiment. The pumping rate was increased to 0.2 l/min in KXTT3 R2. In the PDT-2

test the mass recovery was still relatively low for the flow path KXTT1 R3 to KXTT3 R2, while the flow path KXTT4 R3 to KXTT3 R2 showed a high mass recovery.

Based on the result from the PDT-1 and PDT-2 test it was decided to only use the flow path KXTT4 R3 to KXTT3 R2 in the subsequent PDT-3 test. Further, the test showed that the lowest possible pumping rate to use for pumping in KXTT3 R2 should be 0.2 l/min. The results of the dilution tests performed at the TRUE-1 site indicated that no major change in the boundary conditions has occurred in the two investigated Features A and B.

The objectives of PDT-3 were to test routines for injection, sampling, transport and analysis of radioactive tracer. The test was also made to check that Uranine is a non-sorbing tracer by comparison with tritiated water. The PDT-3 test was conducted as a radially converging test with injection in one section, KXTT4 R3 to KXTT3 R2 using a high pumping flow rate of 0.4 l/min. The injected tracer solution included tritiated water (HTO), two short-lived gamma-emitting tracers ( $^{82}\text{Br}$  and  $^{24}\text{Na}$ ) and Uranine.

Because of the incomplete recovery of tracer in one of the examined flow paths in the PDT-2 experiment another preliminary design test (PDT-4) was performed in KXTT1 R3 to KXTT3 R2. The pumping rate was increased from 0.2 l/min (in PDT-2) to 0.4 l/min. The purpose of the preliminary design test, PDT-4, was to optimise test procedures for STT-1b and to check that tracer mass recovery of the selected flow path was high. The mass recovery for Uranine in PDT-4 was not as high as expected but it was considered high enough for STT-1b to be performed (Andersson et al., 1999a).

## **2.2 Tracer test STT-1 (Task 4E)**

### **2.2.1 Objectives**

The objectives of the TRUE-1 sorbing tracer test STT-1 was to test equipment and methodology for performing tracer test with sorbing radioactive tracers for future stages of the TRUE project. The experiment was also made to increase understanding of transport of sorbing tracers in the studied feature and obtain parameters, which describe retention of tracer transport.

### **2.2.2 Definition and set up**

The tracer test was performed in a radially converging flow geometry with pumping in one borehole section and injection of tracer in another borehole section penetrating Feature A (Andersson et al., 1998b). Pumping was performed in borehole section KXTT3 R2 and tracer was injected in the borehole section KXTT4 R3, see Figure 2-4. The travel distance between the boreholes was 4.68 meters. The injection sections were equipped with a circulation system to rapidly achieve a homogeneous concentration within the section. The volume of the injection section was reduced by inserting volume

reducer (dummies). In total eight tracers, two non-sorbing: Uranine and tritiated water (HTO) and six weakly to moderately radioactive sorbing tracers:  $^{22}\text{Na}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$ ,  $^{137}\text{Cs}$ , were mixed and injected as a finite pulse with a duration of four hours. After four hour of injection the tracer solution was exchanged with unlabelled water. The exchanged procedure lasted for 72 minutes.

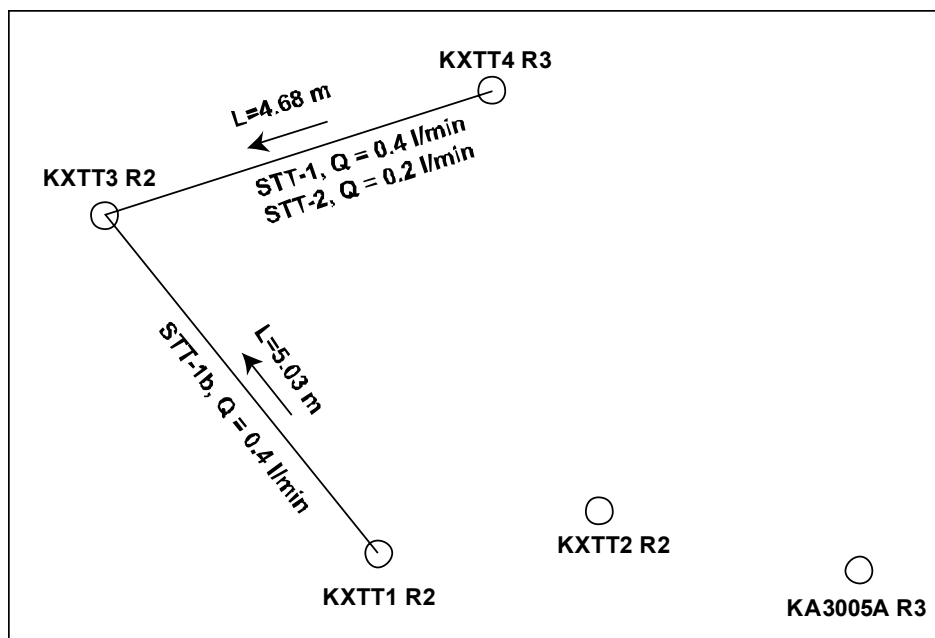


Figure 2-4 Test geometry, pumping flow rates ( $Q$ ) and borehole intersection pattern with Feature A for the tracer tests STT-1, STT-1b and STT-2.

Pumping in the withdrawal section (KXTT3 R2) at a rate of 0.4 l/min started a month prior to the injection in KXTT4 R3. The withdrawal section was sampled with an initial sampling frequency of one sample per 10 minutes during the first two hours and then with a gradually decreasing sampling frequency down to one sample per day after two months.

### 2.2.3 Data base for model predictions

Several deliveries of documents and data were made to the participating organisations and the modelling groups. Three deliveries were made in August 1997 to Mars 1998 containing data on flow and injection concentration for the STT-1. The deliveries also contained data sets for the Preliminary Design Tests. The deliveries included:

- Data set for PDT-1 and PDT-2 (breakthrough and injection curves for Uranine and Amino G) and hydraulic data (head and pump rate) as well as electrical conductivity of pumped water.
- Data set for PDT-3 (injection and breakthrough curves for Uranine) and STT-1 (injection data).
- Data set for PDT-4 (breakthrough curve and injection curves for Uranine) and for STT-1 (breakthrough curves).

## 2.3 Tracer test STT-1b (Task 4E)

### 2.3.1 Objectives

The objectives of the TRUE-1 sorbing tracer test STT-1b was to test equipment and methodology for performing tracer test with sorbing radioactive tracers for future stages of the TRUE project. The experiment was also made to increase understanding of transport of sorbing tracers and to obtain in situ data of sorption from one additional flow path within the studied feature.

### 2.3.2 Definition and set up

The tracer test was performed using a radially converging flow geometry with pumping in borehole section KXTT3 R2 and injection of tracer in borehole section KXTT1 R2, see Figure 2-4 (Anderson et al., 1999a). The travel distance between the boreholes was 5.03 meters. The injection section was equipped with the same circulation system as in STT-1. A solution containing ten different tracers were injected, four non-sorbing (Uranine, HTO,  $^{82}\text{Br}$ ,  $^{131}\text{I}$ ) and six weakly to moderately sorbing tracers ( $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{58}\text{Co}$ ,  $^{99\text{m}}\text{Tc}$ ) as a finite pulse with a duration of 4 hours. After four hour of injection the tracer solution was exchanged in two steps with unlabelled water. The first exchange lasted for 60 minutes and the second exchange, 100 minutes after the end of the first one, lasted for 25 minutes.

Pumping in the withdrawal section (KXTT3 R2) at a rate of 0.4 l/min started in June 1997 prior to the STT-1 test and injection in KXTT4 R3 for the STT-1b test started in November 1997. The withdrawal section was sampled with an initial sampling frequency of one sample per 10 minutes during the first two hours. During the next two hours the sampling frequency was then increased to one sample every 5<sup>th</sup> minute and then gradually decreasing down to one sample per day after two months.

### 2.3.3 Data base for model predictions

Several deliveries of documents and data were made to the participating organisations and the modelling groups. Three deliveries were made in Mars to October 1998 containing data on flow and concentration for the STT-1b test and the final reports on STT-1 and the preliminary design tests (PDT). The deliveries included:

- The final report “Preliminary Design Tests for Tests with Radioactive Sorbing Tracers (PDT-1, PDT-2, PDT-3)” (Andersson, 1998a).
- The draft report “Tracer Tests with Sorbing Tracers, STT-1” (Andersson, 1998b).
- The memo “Radially Converging Tracer Test, RC-3” (Andersson, 1998c).
- Data from the sorbing tracer test STT-1b in Feature A (injection concentration versus time for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{58}\text{Co}$ , pumping rates).

- Data from the radially converging tracer experiment RC-3 (injection concentration of Uranine versus time, Uranine breakthrough in the pumping section versus time, pumping rates).

Finally the experimental results of the breakthrough measurements were distributed in October 1998, containing the following data:

- Breakthrough concentration versus time for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{58}\text{Co}$ .
- Hydraulic head in KXTT1 R2, KXTT2 R2, KXTT3 R2, KXTT4 R3 and KA3005A R3 versus time.

## 2.4 Tracer test STT-2 (Task 4F)

### 2.4.1 Objectives

The objectives of the TRUE-1 sorbing tracer test STT-2 was to test equipment and methodology for performing tracer test with sorbing radioactive tracers for future stages of the TRUE project. The experiment was also made to increase understanding of transport and retention of sorbing tracers in crystalline rock and study the influence of a decreased flow rate on the transport of the tracers compared to STT-1 and STT-1b.

### 2.4.2 Definition and set up

The tracer test was performed using a radially converging flow geometry with pumping in borehole section KXTT3 R2 and injection of tracer in borehole section KXTT4 R3, both penetrating Feature A (Anderson et al, 1999b), see figure 2-4. The travel distance between the boreholes was 4.68 meters. The injection section was equipped with the same circulation system as in STT-1 and STT-1b. A solution containing twelve different tracers were injected, three non-sorbing (Uranine, HTO,  $^{82}\text{Br}$ ) and nine weakly to moderately radioactive sorbing tracers ( $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{99\text{m}}\text{Tc}$ ,  $^{131}\text{Ba}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$  and  $^{137}\text{Cs}$ ) as a finite pulse with a duration of 4 hours. After four hours of injection the tracer solution was exchanged in two steps with unlabelled water. The first exchange lasted for 50 minutes and the second exchange, one hour after the end of the first one, lasted for 40 minutes.

The pumping in the withdrawal section (KXTT3 R2) was decreased from 0.4 l/min to 0.2 l/min eleven days prior to the injection in KXTT4 R3. The withdrawal section was sampled with an initial sampling frequency of one sample per 10 minutes during the first 13 hours and then sampled with a gradually decreasing sampling frequency down to one sample per 96 hours at the end of the test period.

### 2.4.3 Data base for model predictions

Several deliveries of documents and data were made to the participating organisations and the modelling groups. One delivery was made in December 1998 contained data on flow and concentration for the STT-2 test and a technical memorandum on the updated structural model of the TRUE-1 block. The deliveries included:

- The technical memorandum “Updated structural model of the TRUE-1 block and detailed description of Feature A” (Winberg et al., 1998).
- Data from the sorbing tracer test STT-2 in Feature A (injection concentration versus time for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{131}\text{Ba}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$  and  $^{137}\text{Cs}$ , pumping rates).

Finally the experimental results of the breakthrough measurements were distributed in August 1999, containing the following data:

- Breakthrough concentration versus time for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{131}\text{Ba}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$  and  $^{137}\text{Cs}$ .
- Hydraulic head in KXTT1 R2, KXTT2 R2, KXTT3 R2, KXTT4 R3 and KA3005A R3 versus time.

## 3 Modelling approaches

### 3.1 Introduction

A wide range of models and modelling approaches have been applied in Task 4E & 4F. The main focus of the work has been on the transport of sorbing tracers, while the flow modelling generally has received less attention than in the previous tasks. The need to include relatively complex transport processes in the models has in many cases led to the need of simplifying the geometrical description of Feature A. Many of the groups have also performed a great amount of model development during the work with Task 4E and 4F. Thus, the models for prediction of the STT-1 tracer test are in many cases not the same as used for the predictions of STT-1b and STT-2 tests. In Tables 3-1 to 3-2 a summary is made of the flow and transport models used for prediction of the different tests.

The majority of models describe Feature A as a two dimensional planar fracture, where the fracture plane is considered as a continuum extending in two dimensions – *continuum models*. The properties of this continuum (transmissivity, aperture, etc) may either be constant over the fracture plane (*homogenous*) or vary spatially (*heterogeneous*). The spatially varying properties are assigned from a limited number of measurements, which may be used to determine the properties in different parts of the feature - *deterministic modelling*. However, statistical methods are often used to obtain a heterogeneous parameter field, e.g. the transmissivity field. Such a field gives a stochastic representation of the properties of the fracture plane; therefore several realisations are made to obtain statistical measures of output entities. These models are called *stochastic models*. The stochastic fields may be conditioned on measured quantities, e.g. transmissivities and head values.

An alternative approach is to make a discrete representation of the individual features within the rock. In *discrete fracture network models (DFN)* the individual fractures are included in the model in order to address the interconnections between fractures in the rock. The properties of the individual fractures may either be homogenous or heterogeneous. In *channel network models (CN)* the individual flow paths in the rock are modelled. The properties of the flow paths are assigned from statistical distributions defined in such a way that the large scale properties of the rock are maintained.

The modelling of the flow field and the tracer transport is performed in separate steps, usually using different models. The modelling of the flow is for all groups based on the flow equation, while the transport models are either based on the advection-dispersion equation or on particle tracking methods. The transport models include surface sorption, matrix diffusion and sorption.

Table 3-1 Summary of the models for the flow

TOPIC	GRIEPI	JNC/Golder	SKB KTH-ChE	POSI/AVTT 4E	POSI/AVTT 4F	BMW/BGR	SKB KTH-TRUE	Andra/CEA	Nagra/PSI
Type of model	Deterministic continuum model	Discrete fracture network model (DFN)	Stochastic, Discrete Channel Network	Stochastic continuum model	Analytical channel model	Deterministic continuum model	Stochastic continuum model	Analytical & stochastic continuum models	Deterministic continuum model
Process description	Water flow in heterogeneous 2D fracture and homogeneous 3D rock matrix.	Water flow in discrete 3D fracture network.	Water flow in a heterogeneous 3-D channel network	Water flow in heterogeneous 2D fracture.	Water flow through rectangular parallel plate channel	Water flow in heterogeneous 2D fracture	Water flow in a 2D planar fracture with spatially variable aperture.	Water flow in a homogeneous heterogeneous 2D fracture	Water flow in a 2D-homogeneous fracture.
Geometric framework and parameters	Feature A heterogeneous fracture plane, 30x30 m Rock matrix on each side of Feature A modelled as 3D-homogeneous block, 30x30x0.1 m	Modelling of feature A (RC), and zone NW-2* + a highly conductive pathway between KXTT2-KXTT3 (DP) + stochastic background fractures in a 50 m rock block.	Tunnel with niche, Feature A and B. Feature A is extended to the boundaries and Feature B is confined. The size of the modelled rock volume was 30 x 30 x 40m.	Feature A modelled as heterogeneous fracture plane, 15x11 m	Activated flow path(s) represented as single channels	Feature A modelled as heterogeneous fracture plane, 20x20 m. Feature B included but with negligible influence	Feature A is modelled as a 20x20 m planar fracture with spatially variable aperture.	Feature A modelled as a 2D plane. Radial flow field approximated as uniform.	Feature A is modelled as a planar fracture.
Material properties and hydrological properties	Transmissivity (Feature A) Hydraulic conductivity (Rock Matrix)	Transmissivity storativity, aperture	Transmissivity of the Features A and B and rock mass hydraulic conductivity.	Transmissivity Hydraulic aperture based on cubic law.	Number of channels, volume aperture, channel widths, total flow rate through channels and maximum flow velocity	Fracture aperture and hydraulic conductivity	Transmissivity distribution Head and flow distribution	Transmissivity Fracture aperture	Transmissivity Head distribution. $K_{fracture}$ to determine the velocity of the background flow field using head data.
Spatial assignment method	Lognormal transmissivity conditioned to values at boreholes by kriging. Transmissivities at boreholes estimated by trial and error from drawdown of previous tests. Correlation length of 1 m. Hydraulic conductivity assumed to be uniform in the whole rock matrix.	Background fracture: lognormally distributed size and transmissivity from analysis of flow logging in the TRUE-1 borehole array. Feature A: constant, conditioned on borehole transmissivities, POCS generated transmissivity	Lognormal conductances, uncorrelated in space. Not conditioned to measured boreholes transmissivities. Reduced conductance in channels in contact with tunnel.	Lognormal transmissivity with correlation length of 0.4 metres. Calibrated on data from previous tests. Not conditioned to measured boreholes transmissivities. Higher fixed transmissivity around borehole sections.	Constant aperture and width of the channel	Fracture aperture and hydraulic conductivity	2D transmissivity fields conditioned to both transmissivity and head measurements.	4E Constant parameters based on results of preliminary tests used in simulation.	Homogeneous and isotropic transmissivity field.
Boundary conditions	All boundaries: fixed hydraulic heads. Injection sections: fluid flux estimated from decline of measured tracer concentration in injection holes.	Fixed head boundary conditions on the six edges of the model.	Hydraulic head on top, bottom and right side and in tunnel. No flow on other sides on remaining sides. Withdrawal and injection flow rates.	Fixed head boundary condition on the outer boundary of the fracture plane..	Total flow rate through the channels and groundwater transit time	Fixed hydraulic head at top of Feature A and to simulate natural flow conditions, extraction/injection of water in test bore holes.	Constant head on the boundaries.	Constant head on the boundaries. Natural flow field.	Constant injection and pumping flow rates. Constant head far away from the domain of interest.
Numerical tool	FE3M	Fracman/MAFIC	CHAN3D-flow	TFIELD/FEFLOW	(Analytical)	Rockflow-SM2	MODFLOW	CASTEM2000	STREAMLINES
Numerical method	Finite element method	Finite element method	Resistance network, preconditioned conjugated gradient method.	Finite element method	(Analytical)	Finite element method	Finite difference method	Analytical solution Finite element method	Superposition of analytical solution for radial flow and steady-state background flow field.
Output parameters	Head field and flow field.	Hydraulic head, flow in fractures	Head field in each intersection and flow in each channel.	Head field and flow field.	Advection-dispersion breakthrough curve	Head and flow velocity field	Head field and flow field.	Head field and flow field.	Trajectories (streamlines) and velocity vectors.



Table 3-2 Summary of the models for the transport

TOPIC	CRIFPI	JNC/Golder	SKB KTH-ChE	POSAVANTT 4E	POSAVANTT 4F	BMWi/BGR	SKB KTH-TRUE	Andra/GEA	DOE/Sandia	Nagra/PSI
Type of model	Deterministic continuum model	Deterministic continuum model	Stochastic, Discrete Channel Network, Particle tracking	Particle tracking Analytical	Analytical channel model	Deterministic continuum model	Lagrangian stochastic advection reaction	Linear stochastic model	Multirate mass transfer model	Deterministic continuum model.
Process description	Feature A: Advection, dispersion, surface sorption Rock matrix: Advection, dispersion, diffusion and sorption	Advection-dispersion, surface sorption, matrix diffusion and sorption	Advection and matrix diffusion-sorption, spreading due to transport in different channels. Sorption in fracture filling material	Advection, Dispersion due to spatially variable velocity and random component in particle tracking. Surface sorption Matrix diffusion and sorption	Advection, molecular diffusion in the advective flow field, diffusion into fault gauge or stagnant zones, diffusion into rock matrix	Advection, longitudinal and transverse dispersion, diffusion, and sorption in fracture plane, sorption into the matrix	Advection-dispersion due to velocity variation, Diffusion/sorption into rock matrix, Diffusion into stagnant water, Sorption on fracture surface and gouge material	Advection, dispersion Surface sorption Matrix diffusion and sorption	Advection dispersion Mass-transfer by diffusion and sorption	1D-advection, (longitudinal) dispersion, linear sorption, limited 1D-matrix-diffusion. Optional: spatially variable velocities.
Geometric framework and parameters	Feature A a heterogeneous fracture plane, 30x30 m Rock matrix on each side of Feature A modelled as 3D-homogeneous block, 30x30x0.1 m	1 to 9 pathways derived from DFN modelling.	Transport in Channels and diffusion perpendicular to the fracture plane.	Transport in 1D flow paths derived from flow modelling. Unlimited matrix.	Activated flow path(s) represented as single or several parallel flow channels	Feature A modelled as heterogeneous fracture plane, 20x20 m. Feature B included but with negligible influence	Flow path with unlimited matrix.	1D flow path with layered blocks	1D flow path with mass transfer to layered blocks	Feature A modelled as a network of two (independent) fracture families.
Material properties	Fracture aperture, dispersivity, surface related sorption coefficient Rock matrix : Porosity, dispersivity, diffusivity and matrix sorption coefficient	Fracture aperture Path length and width Mean velocity Dispersivity Matrix porosity & diffusivity	Flow porosity calibrated against experimental mean travel time in preliminary test. Flow wetted surface Effective diffusivity, Volume and surface sorption constants. .	Fracture aperture Diffusion coefficient Matrix and surface sorption coefficient	Groundwater transit time, total flow rate and channel width used to calibrate channel aperture	Fracture aperture Dispersivity Diffusion coefficient Distribution coefficient $K_d$	Water residence time and $\beta$ distribution $k_s = \theta[D(1+K_d)]^{1/2}$ increased by a factor. Matrix diffusion and sorption Surface sorption Sorption in the gouge material	Fracture aperture Longitudinal dispersivity Matrix depth Matrix diffusivity Surface and matrix sorption coefficients	Peclet number Mass uptake capacity Mean & SD of log-normal distribution of mass transfer rate Retardation factor Immobile zone Dilution factor	Values for the aperture, extend of the porous rock zone accessible to matrix diffusion, $K_d$ , Dp and $\alpha_L$ from inverse modelling of the STT1 tracer test.
Spatial assignment method	Constant parameters based on results of preliminary tests used in simulation.	Constant parameters based on results of preliminary tests used in simulation.	Channel volume derived from conductance using cubic law.	Transport aperture proportional to hydraulic aperture from variable transmissivity	Constant aperture and width of the channel	Constant parameters in fracture	Spatially variable velocity field in fracture	Constant parameters in fracture	Constant parameters in fracture	Constant aperture of fractures.
Boundary conditions	Pulse injection, breakthrough curves calculated by convoluting with measured injection. No mass flux on surrounding boundaries	Tracer injection flow rate and concentration.	Tracer injection flow rate and concentration.	Pulse injection, breakthrough curves calculated by convoluting with measured injection curve.	Pulse injection, breakthrough curves calculated by convoluting with measured injection curve.	Tracer injection flow rate and concentration	Injection flow rate and injection data (LaSAR)	Imposed concentration at the injection borehole, dispersive flux equal to zero at the pumping borehole	Tracer injection flow rate and concentration.	Time-dependent flow boundary condition upstream, zero dispersive flux boundary condition down-stream.
Numerical tool	FERM	LTG	CHAN3D-transport	BTSIMU-MDIFF	Analytical	Rockflow- TM2	PATHLINE, LaSAR	CASTEM2000	STAMMT-L	PICNIC
Numerical method	Finite element method	Laplace Transform Galerkin	Particle-following technique	Particle tracking method Analytical	Analytical	Finite element method	Particle tracking method	Mixed hybrid finite element method	Laplace transformation technique for injection and Dirac pulse.	Laplace transformation technique for injection and Dirac pulse.
Output parameters	Breakthrough curves.	Breakthrough curves for actual injection and for Dirac pulse. Cumulative curves.	Breakthrough curves	Breakthrough curves	Breakthrough curves	Breakthrough concentration distribution	Water residence time and $\beta$ -distribution Breakthrough curves	Breakthrough curves, mean and standard deviation	Breakthrough curves	Breakthrough curves.

## 3.2 Approaches applied by the modelling teams

### 3.2.1 CRIEPI

The Central Research Institute of Electric Power Industry (CRIEPI) of Japan participated in Tasks 4E and 4F with the specific modelling objective of deepening their understanding of migration phenomena of sorbing solutes in a fracture. Furthermore, they wanted to assess the usefulness of the numerical codes developed for prediction of such phenomena. The modelling group performed predictive modelling of Task 4E and Task 4F. After the experimental results were delivered also an evaluation of their model was made including fitting the experimental results (Tanaka et al., 2000).

Feature A was considered as an isolated fracture described as a flat square with a side of 30 m. The flow in the fracture was solved with the flow equation and the tracer transport using the advection-dispersion equation. Dispersion and diffusion within the fracture plane was taken into account. For the predictions of STT-2 also diffusion into the rock matrix was considered. The calculations were made with the Finite Element method on a mesh refined in the central part where the boreholes were located. The number of elements was about 4000 for the two-dimensional simulations of STT-1 and STT-1b and about 23 000 for the three-dimensional simulations for STT-2.

The transmissivity field of Feature A was assumed to have a lognormal distribution. The transmissivities at the borehole intersections (KXTT1 - KXTT4) were obtained by minimising the error of predicted and observed drawdown in the previous tracer tests. The transmissivity at KA3005A was taken from the flow- and pressure build-up test. The transmissivity field was estimated by kriging on the basis of the transmissivities of the five borehole intersections with an exponential model for the spatial correlation and a correlation length of 1 meter. A fixed hydraulic head was set on the surrounding boundaries. The magnitude and direction of the gradient was estimated from head measurements before the start of PDT-3.

The mass flux in the injection section was calculated based on the decline of the concentration of the two tracers Uranine and Amino G Acid in the injection section. The product of tracer concentration and the fluid flux was input as the mass flux of tracer.

#### *Tracer test STT-1*

The predictions of STT-1 were made using the two-dimensional model. The fracture aperture and longitudinal dispersivity was obtained by fitting the Uranine breakthrough in PDT-3. To estimate surface sorption, the geometric mean of laboratory  $K_a$ -values were used (Andersson et al., 1997), based on the geometric surface after 1 day and 14 days. The predicted breakthrough curves were found to reach a higher maximum value than the experimental curves. The predicted maximum value was also reached much earlier than in the experiment.

### *Tracer test STT-1b*

The predictions for STT-1b were made with the same model, transmissivity distribution and boundary conditions as for STT-1. The fracture aperture and longitudinal dispersivity were derived from fitting the breakthrough in PDT-4. The surface sorption coefficients ( $K_a$ ) for Na-22, Sr-85 and Rb-86 were obtained from the evaluation of the results from the STT-1 test. These  $K_a$ -values were between 3.4 and 4 times higher than the  $K_a$ -values derived from laboratory data that were used in the prediction of STT-1. The predicted curve showed reasonable agreement with the measured curve, but the tail tended to decline much faster than in the experiment.

### *Tracer test STT-2*

The three-dimensional model was used for the predictions of STT-2, thereby including the effect of matrix diffusion and sorption. The transmissivity distribution in the fracture and the boundary conditions were the same as in the previous predictions. The fracture aperture and longitudinal dispersivity was obtained by fitting the Uranine breakthrough in PDT-2. The effective diffusivities in the rock matrix, the surface sorption coefficients and matrix sorption coefficients were obtained by fitting the results of the STT-1 experiment using the three-dimensional model. The predicted breakthrough curves showed a higher maximum value that was reached earlier than in the experimental curves.

## **3.2.2 JNC/Golder**

The modelling team from the Japanese Nuclear Cycle Development Institute (JNC) and Golder Associates has participated in Tasks 4E and 4F with the purpose of improving the understanding of flow and transport of sorbing radionuclides in discrete fracture networks with the focus on transport and the role of fracture connectivity. Special issues addressed were the role of flowpath networks and the effect of immobile zones (Dershowitz et al., 2000).

The JNC/Golder group has based their predictive calculations on stochastic discrete fracture network models (DFN). The DFN model covers a 50 x 50 x 50 m block containing a limited number of deterministic features in a stochastically generated network of fractures. The present model included Feature A, Feature A\* (a high permeability feature between KXTT2 and KXTT3) and Feature NW-2, and about 350 stochastic background fractures. Flow simulations with the DFN-models provided simulated drawdown and transport pathways. The transport of non-sorbing and sorbing tracers in these pathways have been simulated using a variety of transport models.

### *Tracer test STT-1*

For the STT-1 predictions, multiple DFN realisations of the geologic conceptual model containing Feature A were generated. Three models of heterogeneity within Feature A were tested. In the first a constant transmissivity was used, set somewhat lower than previously used in the predictions of Task 4D. In the second the transmissivity field was conditioned to borehole transmissivities and interpolated between the known values. In

the third POCS-model the transmissivity field conditioned to known values in boreholes and a fractal roughness between boreholes was assigned. The three models did not give significantly different results in the calibration and only the model with constant transmissivity and the POCS-model were used for the predictions.

Flow simulations of the DFN models provided simulated drawdown and, via particle tracking, simulated non-sorbing tracer breakthrough curves. Nearly 100 simulations were made to calibrate the transmissivity and transport aperture to fit the results of the PDT-1, PDT-2 and PDT-3 tests. The calibrated model was then conditioned on the PDT-3 test. Of the 50 realisations performed 10-20 gave acceptable results of drawdown and breakthrough for non-sorbing tracers compared with the PDT-3 test. The accepted realisations were then used to predict STT-1.

Solute transport was simulated by particle tracking using the MAFIC model. Retardation of sorbing tracers was modelled by estimating a relative velocity for each tracer based on the surface sorption coefficients determined from the laboratory experiments (Andersson et al., 1997). The relative velocity was 100% for Uranine, 80% for Na, Ca and Sr, 10% for Rb and Ba and 1% for Cs. Tracer breakthrough was calculated by injecting about 10 000 particles in a step-pulse. The tracer injection in STT-1 was simulated by slug superpositioning of the breakthrough curve with the measured injection concentration curve.

The experimental breakthrough curves showed an earlier initial breakthrough and a more pronounced tailing than the predicted curves indicating the possible importance of matrix diffusion or other immobile zone exchange processes. Thus, the STT-1 evaluation focussed on the effect of these processes testing different conceptual models.

#### *Tracer test STT-1b*

Based on the evaluation of the STT-1 predictions, the modelling strategy was somewhat revised for the predictions of STT-1b. In order to evaluate the importance of multiple pathways a Laplace Transform Galerkin solute transport model (LTG) was applied.

As a first step a DFN simulation with MAFIC was made to simulate the drawdown and non-sorbing tracer breakthrough in the PDT-4 test. Several modifications were made in the DFN model for the predictions of the STT-1b tracer test. In this case the transmissivity field of Feature A was conditioned to the measured values at the boreholes and a refined mesh was used to avoid problems during the particle tracking. A lower transmissivity was used for the background fractures in order to reduce the flow through the background fracture network. As this made the storativity of the background features less accessible, the storativity of the background features as well as of Feature A was increased.

In the next step a single flowpath and a two flowpath model was set up with LTG. These models were calibrated to fit the non-sorbing tracer breakthrough of PDT-4. Although the two path model did not provide a significantly better fit than the one path model it was still considered as the preferred model. The reason being an unrealistically high porosity in the one path model and that the experience from the STT-1 evaluation showed that a better fit for sorbing tracers could be obtained with a two path model.

Tracer transport was evaluated taking into consideration surface sorption and matrix diffusion and sorption. Experimental values of surface sorption (Crushed material, geometric surface, 1 day) and matrix sorption (Äspö diorite) were used (Byegård et al., 1995), except for Co where field values from other sites were applied.

#### *Tracer test STT-2*

The model used for prediction of STT-2 was essentially the same as that used to predict the previous tracer tests. However, in this case a pipe network for the transport modelling consisting of nine pipes was derived from the DFN-model. The nine pathways were based on background fracture intersections with Feature A. Seven of the pathways remain in Feature A between the two wells, while the remaining two go through background fractures near the well. The basis for using multiple pipes was the complex form of the breakthrough curve of PDT-2.

Solute transport in the nine pathways was modelled using the LTG-model. The model takes into consideration advection-dispersion in multiple pathways, surface sorption, diffusive exchange between mobile and immobile zones, matrix diffusion and sorption. Calibration was made to the PDT-2 breakthrough curve by adjusting fracture aperture, matrix porosity and diffusion distance of the pathways.

As a result of the evaluation of the previous tracer tests the surface sorption coefficients for Na, Sr and Rb were increased about 2.5 times compared to the values used for the STT-1b predictions. For Ca, Br and Cs the values taken from Andersson et al. (1997) were retained. The value for Ba was taken from Ohlsson and Neretnieks (1995). The matrix sorption coefficients were derived from the surface sorption coefficients, which resulted in somewhat higher values for the more sorbing radionuclides than previously used.

### **3.2.3 SKB/KTH-ChE**

The Royal Institute of Technology/Department of Chemical Engineering (KTH-ChE) of Sweden on assignment of the Swedish Nuclear Fuel and Waste Management Co (SKB) has participated in Tasks 4E and 4F with the purpose of increasing the knowledge about transport of sorbing species in fractured rock (Moreno, 2001). An additional purpose was testing of the model CHAN3D by applying it to experiments with sorbing species.

The modelling team focussed on the flow and transport in a network of flow paths (channels) in the fractured rock volume using the code CHAN3D (Gylling et al, 1999). The code is based on the Channel Network model developed by Moreno and Neretnieks (1993), where flow and transport is presumed to take place in a three-dimensional network of channels. The structure of the grid is cubical, with six channels meeting at the connections. The length and hydraulic conductivity of the individual channels were described by a hydraulic conductance, assigned from a statistical distribution. The transport was simulated by a particle-following technique where the total residence time of a particle is the sum of its residence time in the channels it has passed through. In order to estimate the residence time for non-sorbing tracers a channel volume is needed. The effect of diffusion into the rock matrix and sorption was simulated by assigning the

residence time of a particle in the individual channels from a distribution derived from an analytical equation for advection with matrix diffusion and sorption. In this case also the flow wetted surface must be provided. Hydrodynamic dispersion within the channels was neglected, only matrix diffusion and sorption and the presence of different flow paths will thus cause dispersion.

The SKB/KTH-ChE team has modelled a rock block of 30 x 30 x 40 metres including part of the tunnel, the niche, the boreholes and Features A and B. The discrete features were described by assigning a specific conductance distribution to the channels belonging to a particular feature. Feature A was extended to the boundaries while Feature B was considered as a confined plane. A channel length of 0.7 metres was used giving a network of 350 000 channels.

A constant hydraulic head was assigned at the top, bottom and the vertical side away from the tunnel. On the opposite vertical side the part containing the tunnel and the niche was assigned the hydraulic head in the tunnel, while the remainder of that side was treated as a no flow boundary. Also the vertical sides perpendicular to the tunnel were treated as no flow boundaries.

The conductance of the channel members was assumed log-normally distributed and non-correlated in space. The mean values of the conductance distribution of channels belonging to Features A and B were assigned from measured transmissivities and calibrated to fit drawdown of preceding preliminary tracer tests. No conditioning of the transmissivity was made at the intersecting boreholes. The mean conductance of the channels in the surrounding bedrock was calculated from the hydraulic conductivity of the rock mass. A lognormal standard deviation of 1 was used for all features based on measurements at the Äspö site (Gylling et al., 1994). The conductance of the channels connecting to the tunnel was reduced by a factor of 10 to simulate the skin effect. The flow porosity (total volume of the channels included in Feature A) was matched against the results of the preliminary design tests, see below. The volumes of the individual channels were estimated assuming that the conductance is proportional to the cube of the channel aperture. The channels in the rock were assumed to have lower flow porosity than those in the features. The specific flow wetted surface was estimated to be  $1 \text{ m}^2/\text{m}^3$ , which for a channel length of 0.7 m corresponding to a channel width of 0.25 m.

#### *Tracer test STT-1*

The preliminary tracer tests PDT-1 – PDT-3 were used to calibrate the model. The conductance of the channels belonging to Feature A was varied in order to match the drawdown observed in these tests. The reduction of the conductivity in the channels intersecting the tunnel was varied in order to match the observed tracer recovery. The void volume was calibrated to fit the breakthrough time for Uranine in the PDT-3 test.

The matrix sorption coefficients and diffusion coefficients were taken from the provided laboratory data (Andersson et al., 1997).

### *Tracer test STT-1b*

No recalibration was made of the channel conductances for the predictions of STT-1b. However, the void volume of the channels was calibrated to fit the breakthrough time for Uranine in the PDT-4 test.

In the evaluation of STT-1b it was found that the predicted travel times for the sorbing tracers were considerably shorter than those observed in the experiment. The cause of this difference was studied and several possible causes for the difference were identified:

- Either the diffusion and/or sorption into the rock close to the fracture is more prominent than was evaluated from the laboratory data.
- The water flow rate through which the tracers were transported was smaller than the average value, which would increase the efficiency of matrix diffusion and sorption.
- Sorption occurs also on fracture surfaces, filling material or gauge material.
- Diffusion occurs into zones with stagnant water, which may be important if the transport paths are narrow and the fracture aperture is large.

It was found that in order to simulate the experimental results the product of the matrix sorption coefficient and matrix diffusivity should be 900 times larger than the value obtained from the laboratory data (Andersson et al., 1997). Alternatively, the flow rate in the part of the fracture where transport occurs should be a factor 30 lower than the average flow rate.

### *Tracer test STT-2*

The preliminary tracer test PDT-2 was used to calibrate the model. The conductance of the channels belonging to Feature A was varied in order to match the drawdown observed in PDT-2. The void volume was adjusted to fit the breakthrough in PDT-2. The reduction of the conductivity in the channels intersecting the tunnel was varied in order to match the observed tracer recovery.

In an evaluation of the predictive modelling various explanations for the deviations between predicted and observed breakthrough curves were investigated. This evaluation is further discussed in Chapter 5.

## **3.2.4 Posiva/VTT**

The modelling team from Posiva Oy and VTT Energy of Finland participated in the task for the purpose of increasing the knowledge of flow and transport in a heterogeneous single fracture as a basis for performance assessment. A carefully conducted set of tracer tests in a hydraulically well characterised fracture with accurately measured source terms and varied pumping was expected to reveal essential features of the flow and transport processes. A main issue was how the flow heterogeneity (channeling), especially the flow rate distribution over the fracture plane, influenced the interaction of

transported solutes with the fracture walls in various parts of the fracture. This is a prerequisite for matrix interactions.

The Posiva/VTT team used different modelling approaches to predict the tracer experiments (Poteri, 2000). Various analytical expressions have also been used to evaluate the importance of various transport processes. Two different conceptual models were applied to predict the three tracer tests. The first two tests (STT-1 and STT-1b) were modelled assuming transport in a two-dimensional heterogeneous fracture, while the last test (STT-2) was modelled assuming transport in flow channels. In both cases the breakthrough curve for a pulse injection of a non-sorbing tracer was first simulated. The non-sorbing tracer breakthrough was divided into a discrete set of streamtubes. Each streamtube was assumed to have identical properties, but with a different flow-rate. The effect of sorption and matrix diffusion was evaluated for each streamtube and the total release was evaluated by integrating the release from the individual streamtubes. Finally, the predicted tracer release was evaluated by convolution with the experimental injection curve.

Processes considered in the modelling were advection, Taylor dispersion, surface sorption, diffusion into zones of stagnant water, diffusion into the rock matrix with subsequent sorption.

#### *Tracer tests STT-1 and STT-1b*

The two-dimensional heterogeneous fracture plane used in STT-1 and STT-1b was modelled using the stochastic continuum approach (Poteri, 2000). No intersecting fractures or background fractures were included. The hydraulic head field in Feature A was calculated by solving the flow equation in two dimensions. The modelled plane had the dimensions 15 x 11 meters, which was judged to be large enough to have fixed head boundary conditions at the outer edges. The grid consisted of about 15 000 equally sized elements with a side of about 0.1 m. An isotropic transmissivity field was generated based on a lognormal transmissivity distribution and a spherical correlation function. The transmissivity field was not directly conditioned to the measured borehole transmissivities.

The finite element code FETRA was used to solve the hydraulic head field using linear two-dimensional elements. The boundary conditions were extrapolated from head values measured before the PDT-3 test. The transmissivity fields used in the transport calculations were calibrated against drawdown data from ten different tracer tests previously performed in Feature A. Calculations were made with a total of 799 realisations of the transmissivity field. Based on the results of the preliminary tracer test a standard deviation of the log transmissivity in the range  $\sigma = 1.5 - 2$  was expected. However, as was the case for the simulations for Tasks 4C and 4D the head field solution became unreliable using such high standard deviation. Therefore a fixed standard deviation of  $\sigma = 1$  was used. The mean transmissivity was calibrated to fit the mean drawdown in the injection holes of all radial tests. This gave a mean log transmissivity of  $\mu = -6.8$ , which is close to the value obtained in the interference test.

The 30 realisations that had the least sum of the squared difference between measured and simulated drawdown were selected for the predictive modelling. This approach



gives a conditioning of the transmissivity field within a distance from the boreholes corresponding to the correlation length. Furthermore, the part of the fracture closer than 0.1 metres to the pumping hole was assigned a high transmissivity value ( $5 \cdot 10^{-5} \text{ m}^2/\text{s}$ ) in order to ensure a sufficient hydraulic conductivity between the boreholes and the rest of the fracture plane.

Tracer transport was calculated using the particle tracking method. The water velocity was calculated with a parallel plate model (cubic law) using the local transmissivity and the gradient of the hydraulic head estimated by a bicubic fit of the solved hydraulic head field. The tracer particle velocity was calculated by multiplying the water velocity by a factor of 11, obtained from the calibration to the results of the PDT-3 test. Dispersion of the tracer due to hydrodynamic dispersion in the fracture plane was taken into account. The dispersion caused by molecular diffusion was estimated to be considerably smaller than that due to hydrodynamic dispersion. Hydrodynamic dispersion should in principle be modelled explicitly by the heterogeneous flow field. However, it was judged that the description of the variable flow field was not detailed enough to simulate the local scale variation flow velocities in order to obtain a reasonable value for the dispersion. Thus, in the predictive modelling hydrodynamic dispersion was modelled by applying a dispersion coefficient of  $10^{-4} \text{ m}^2/\text{s}$ , obtained by fitting the results of the PDT-3 test. The dispersion was described by adding a random component to the particle displacement.

The breakthrough curves were calculated for a Dirac pulse injection using 2000 tracked particles. The non-sorbing tracer breakthrough was divided into a discrete set of streamtubes. Each streamtube was assumed to have identical properties, but with a different flow-rate. The effect of sorption and matrix diffusion was evaluated for each streamtube and the total release was evaluated by integrating the release from the individual streamtubes. The sorption parameters  $K_a$ ,  $K_d$  and the diffusivities were selected from the laboratory data provided to the modelling groups (Anderson et al., 1997). The experimental breakthrough curves were simulated by convoluting the calculated pulse response with the measured time series of the tracer concentration in the injection boreholes.

#### *Tracer test STT-2*

An alternative modelling approach was applied to the STT-2 tracer test, which only looked at transport and did not predict the drawdown. This approach is based on the assumption that only a few channels dominate the transport. The water velocity in such a channel will due to variations in aperture vary over the width of the channel. These velocity variations will cause a dispersion of the tracer, analogous to Taylor dispersion. The Taylor dispersion due to velocity variations over the aperture of the channel was considered to be of little importance since molecular diffusion will even out the concentration gradient perpendicular to the flow direction in a short time. In the model the velocity profile over the width of the fracture was assumed to vary linearly from a maximum value at the centre to zero at the edges. The average concentration over the channel width was solved analytically.

In a first step the breakthrough curve for a pulse injection of a non-sorbing tracer was simulated. The effect of diffusion into stagnant zones, sorption and matrix diffusion was evaluated using the same method as for the fracture model. The non-sorbing tracer

breakthrough was divided into a discrete set of streamtubes and the effect of diffusion and sorption was evaluated for each streamtube. Total release was evaluated by integrating the release from the individual streamtubes. Finally, the predicted tracer release was evaluated by convolution with the injection curve.

For STT-2 the transport parameters were fitted to the results from the STT-1 test rather than obtained from the laboratory data. The surface sorption retardation factor was calculated from the rising slope of the STT-1 breakthrough curve. The  $u$ -parameters, describing the effect of matrix diffusion and sorption and diffusion into zones with stagnant water, were fitted to the STT-1 breakthrough curves. The fitted  $u$ -parameter was adjusted to the lower flow rate in the injection section during STT-2.

### 3.2.5 BMWi/BGR

The Federal Institute of Geosciences and Natural Resources (BGR) supported by the Federal Ministry for Economics and Technology (BMWi) of Germany has participated in the Task 4E/4F modelling work with the purpose of understanding transport mechanisms for radioactive solutes in fractured rock and testing numerical models developed for this purpose. An additional purpose of participating was the possibility to exchange experience with international partners, e.g. from the in-situ experiments performed at the Grimsel site in Switzerland where BMWi/BGR has participated. The modelling group especially wants to test their knowledge about sorption of tracers in fractured rock, for example to what extent the  $K_d$ -parameter is suitable for describing the sorption reactions.

The geometrical model of the features within the TRUE-1 block used in Task 4E and 4F (Shao and Liedtke, 1999) was basically the same as used in Tasks 4C/4D (Liedtke and Shao, 1997), where Features A and B have been treated as two-dimensional planar structures. However, the hydraulic influence of Feature B on Feature A was found to be negligible, due to the large difference in transmissivity. Feature A was modelled using a uniform grid with dimensions 20 x 20 m with varying hydraulic conductivity and fracture aperture. For the STT-1 predictions a 2D-fracture model was used. In the evaluation of the experiment, the grid describing the feature was extended to a 3-dimensional fracture-matrix model, in order to describe matrix diffusion and sorption. For STT-1b and STT-2 the 3D-model was simplified so that each 2D fracture element was connected to a 1D matrix element attached perpendicular to the fracture plane. The depth of the fracture matrix was 0.1 m.

The flow in the feature was obtained by solving the flow equation. A heterogeneous model was used where different parts of the fracture were assigned hydraulic properties by calibrating to the results from previous experiments using an iterative trial and error technique, i.e. not a statistical procedure. The model of Feature A was twice the experimental area, which was judged to be large enough not to be influenced by the pumping. The natural flow field was simulated by setting a fixed head at parts of the model boundaries, while the remainder of the boundaries had no flow. The boundary conditions used were the same as in Tasks 4C/4D. The injection and pumping was simulated by assigning a prescribed flow rate at the location of the wells.

The tracer transport was simulated with the advection-dispersion equation using the calculated water velocity field from the flow model. Hydrodynamic dispersion and molecular diffusion were described as a Fickian process. The finite element discretisation (0.5 – 1 m) was in the same order as the dispersion lengths used (0.6 – 0.9 m). Diffusion into the rock matrix was included in the matrix models. The injection of tracer was modelled using a time dependent concentration at boundary representing the injection segments corresponding to the experimental concentrations.

#### *Tracer test STT-1*

Two meshes were used in the predictions of STT-1 with different spatial distribution of the hydraulic conductivity. The hydraulic conductivity in Mesh 1 was calibrated against the hydraulic data from all the previously performed dipole tests while Mesh 2 was calibrated only using results from the tracer tests with the same test configuration as STT-1 (DP-6, PDT-2 and PDT-3). The transport parameters were calibrated using the breakthrough of Uranine from previous tracer tests, with focus on the tracer tests performed in the same configuration. In the predictive calculations sorption was modelled as equilibrium sorption on material in the fracture. The  $K_d$ -values were varied within the range obtained for Äspö diorite from the laboratory experiments (Andersson et al., 1997).

The evaluation of the predictions showed that for non-sorbing and weakly sorbing tracers the experimental results were within the predictions made with the range of  $K_d$ -values reported from experiments. However, for moderately sorbing tracers (Cs-137, Rb-86) no satisfactory results could be found even using a wide spectrum of  $K_d$ -values. In order to interpret the results for sorbing tracer a matrix model was introduced, where 3-D elements representing the rock matrix were connected to the 2D fracture elements. Transport was assumed to occur by advection-dispersion in the fracture and diffusion in the matrix. Sorption was assumed to occur both on the fracture surfaces and in the rock matrix.

#### *Tracer test STT-1b*

Before the prediction calculations for STT-1b, the model was calibrated against the hydraulic data and tracer transport information obtained from the PDT-4 test, performed with the same configuration. The hydraulic conductivity, the fracture aperture and the effective porosity in the fracture near borehole KXTT1 were varied. The calibrated model was tested by simulating the breakthrough of Uranine in the PDT-1, PDT-2 and PDT-4 tests. Based on the experience from the STT-1 test, the fracture model was used to predict the breakthrough of non-sorbing tracers and a matrix model to predict the breakthrough of moderately sorbing tracers. However, since the 3D-model used for STT-1 was very demanding in terms of computer capacity a different approach was used. In the new model – the Brush model – 1D finite elements representing the matrix were attached to each 2D fracture element. The cross-sectional area of the 1D elements was set to be equivalent to the corresponding fracture element. Due to symmetry only half of the fracture aperture was considered.

In the evaluation of the STT-1 predictions it was found that the prediction of the non-sorbing and weakly sorbing tracers were satisfactory, while the  $K_d$ -values for the more sorbing tracers needed to be adjusted to obtain a reasonable fit.

#### *Tracer test STT-2*

The predictive modelling of STT-2 was performed using the same model as for STT-1b, except for a slight modification of the dispersivity done with respect to the modelling of PDT-2. The modelling group also performed a model variation in order to evaluate the influence of a fracture intersecting KXTT4 R3 subparallel to Feature A. The conclusions were that the subparallel fracture caused a slight reduction in dispersivity, but did not have any major influence on the shape of the breakthrough curve. The predictions for STT-2 were therefore based on the single fracture model.

### **3.2.6 SKB/KTH-TRUE**

The modelling team from Royal Institute of Technology/Water Resources Engineering of Sweden and SKB was part of the TRUE Project team. The predictions for Tasks 4E/4F are a part of the predictions/evaluations made within the TRUE programme (Cvetkovic et al., 2000). The SKB/TRUE team especially wished to address the possibility to increase the understanding of mass transfer processes in Feature A.

Feature A was modelled as a single two-dimensional plane with dimensions 20 by 20 metres. The flow in the feature was described by the two-dimensional flow equation using a spatially variable transmissivity with an assumed distribution and correlation length (stochastic continuum approach). The calculations were performed using the computer code MODFLOW on an equidistant mesh with an element size of 0.4 meters. The transmissivity field was conditioned on measured transmissivity values and steady-state heads prior to and during the pumping for the tracer test RC-1. A constant head of -46.5 m was set at the boundaries. A spatial distribution with a mean  $m_Y = -7.7$ , a variance of  $\sigma^2_Y = 0.4$  and a correlation length of 1 metre was used as a starting point of the conditioning. A spatially variable aperture was derived by assuming that transmissivity and aperture are related through the cubic law.

Transport was assumed to take place in a single fracture with spatially variable aperture. The transport in the feature was described by a Lagrangian travel time approach where surface sorption, matrix diffusion and sorption and diffusion into stagnant zones affect the transported solute. Dispersion within a single streamline was not considered, but will be due to variation between different streamlines.

In the Lagrangian Stochastic Advection Reaction (LaSAR) framework two random parameters are introduced  $\beta$  and  $\tau$ , which depend on the aperture heterogeneity. The  $\beta$ -parameter which is a flow-dependent parameter controlling the tracer diffusion into the rock matrix and is an integral entity describing the ratio flow wetted surface to water flow rate along a streamline. The  $\tau$ -parameter is the water residence time.

### *Tracer test STT-1*

For the predictions of the STT-1 test the transport times were evaluated using particle tracking in the velocity field obtained with the spatially variable transmissivity and aperture. The transport times were calibrated to the experimental transport times obtained in the RC-1 tracer test using a calibration factor of 9. The number of particles was 100. Transport modelled using analytical solution for pulse injection with surface sorption, matrix diffusion and sorption. The simulated breakthrough curves were obtained by convolution with injection curves for the different tracers. An effective value of the  $\beta$ -parameter was determined as the expected value for each realisation.

Surface sorption coefficients ( $K_a$ -values) were taken from laboratory measurements (14 d, geometric surface). Matrix sorption and diffusion data were taken from the through diffusion experiments on Äspö diorite. Matrix sorption was determined to be of minor importance for the present case and thus only the effect of surface sorption was considered in the predictions.

In the evaluation of the STT-1 experiment it was found that the predictions for the more strongly sorbing tracer differed considerably from the experimental results.

### *Tracer test STT-1b*

The same numerical tools as in the STT-1 simulations were used. However, for the predictions of the STT-1b tracer test kinetic sorption on fault gouge and diffusion into stagnant zones was introduced. A linear relationship between  $\beta$  and  $\tau$  was used, derived from calculating the correlation between  $\beta$  and  $\tau$  in multiple realisations. The cross-section area for diffusion into stagnant zones was derived assuming the pathline width corresponding to the borehole diameter. The surface and matrix sorption coefficients and diffusivities were taken from the laboratory measurements, while the sorption coefficients for the gouge material and the rate constant for the kinetic sorption were derived from the evaluation of the STT-1 test.

In the evaluation of STT-1 and STT-1b the water residence time distribution was derived by deconvolution of the breakthrough curve for the non-sorbing tracer HTO assuming an inverse Gaussian distribution. The sorbing tracer breakthrough was derived from the water residence time distribution using a calibration factor for the matrix diffusion and sorption and by adding sorption to the gouge material. The calibration factor for matrix diffusion and sorption can imply higher values for the diffusivity, or of the matrix sorption coefficient. The calibration factor needed to enhance matrix diffusion and sorption was found to vary between 40 and 50 for the tracer in STT-1 and between 32 and 34 for the tracer in STT-1b.

### *Tracer test STT-2*

In the predictions of the STT-2 tracer test, the water residence time distribution was derived by calibrating the calculated breakthrough against the experimental data from PDT-2, assuming an inverse Gaussian distribution. From the evaluation of STT-1 it was found that the effect of matrix diffusion and sorption needed to be increased in order to

explain the experimental data. The enhancement factor  $f$  and the parameters for kinetic sorption on the gouge material derived for STT-1 were used for the prediction of STT-2.

The SKB/KTH-TRUE team has performed an extensive evaluation of the tracer tests as a part of the TRUE work. This evaluation will be further discussed in Chapter 5.

### 3.2.7 ANDRA/CEA-DMT

The Agence Nationale pour la Gestion des Déchets Radioactifs / Commissariat à l'Énergie Atomique Direction des Réacteurs Nucleaires-Departement de Mécanique et de Technologie (ANDRA/CEA-DMT) has participated in the Task 4 modelling work presenting predictive results for the STT-1 (Mouche et al., 1998) and STT-2 (Grenier and Mouche, 1999) tracer tests. No predictions were made for STT-1b.

The ANDRA/CEA-DMT team has modelled the Feature A as a two-dimensional fracture using a deterministic approach. Both analytical and numerical models were used. The numerical model is based on the mixed hybrid finite element code CASTEM2000.

#### *Tracer test STT-1*

In the predictions of the STT-1 tracer test Feature A was assumed to be homogeneous with a log transmissivity of -7.4, a fracture aperture of 1.4 mm and a dispersion length of 1.6 meters based on the PDT-2 and PDT-3 tracer tests.

The approximation of Lenda and Zuber (1970) was used for the transport model, whereby the breakthrough curve in a radially converging flow field can be approximated by the breakthrough curve in a uniform flow field with the same travel time. The approximation was made, due to numerical problems solving the transport equation in a radially converging flow field. Based on the pumping rate and the fracture aperture, the mean flow velocity was calculated as  $3.2 \cdot 10^{-4}$  m/s. The transport model takes into account surface sorption and matrix diffusion and sorption. The surface sorption and matrix sorption coefficients were taken from laboratory data (Andersson et al., 1997). The model was checked against the breakthrough curve of the PDT-3 test, but it was not possible to satisfactorily simulate the large tailing observed in the experimental breakthrough curve. However, due to time constraints a calibration could not be done and the parameter values were kept for the prediction of the STT-1 non-sorbing and sorbing tracers.

#### *Tracer test STT-2*

A somewhat different approach was used for the predictive modelling of the STT-2 test. The purpose was to investigate the reason for the high dispersivity observed in the flow path used for STT-1 and STT-2, which could be caused by the presence of multiple pathways or to matrix diffusion effects. In a first step, the effect of the natural gradient and heterogeneity in the transmissivity field was evaluated. Calculations of the flow field using the numerical code were done for cases with a homogeneous transmissivity field with and without the natural flow field. Comparing the flow paths obtained for the

two cases it was found that the natural flow field was of secondary importance. In the second step, kriged maps of heterogeneous transmissivity fields were created. In the first cases kriging was based only on measured transmissivity data and in the second case on transmissivity data and natural flow head data. For the second case the flow paths were strongly affected by the heterogeneity.

The transport model considered advection, dispersion and enhanced matrix diffusion due to fracture gouge material, altered crystalline rock, stagnant pores or the presence of flowpaths increasing the effective contact area between mobile and immobile water zones. The predictions of tracer breakthrough were made using a uniform flow field based on the approximation of Lenda and Zuber. Preliminary evaluations of the PDT-3 tracer breakthrough using an analytical model indicated that diffusion into matrix zones could account for a large part of the tailing observed in the experiments.

For the predictions of the STT-2 tracer breakthrough values for the dispersion length, matrix porosity and matrix diffusivity were obtained by calibrating on the PDT-3 breakthrough curve. Data for surface sorption and matrix sorption were taken from the laboratory experiments, but assuming an increased area for matrix diffusion and surface sorption. Predictions were only made for non-sorbing and weakly sorbing tracers.

### **3.2.8 DOE/Sandia**

The United States Department of Energy (DOE) and Sandia National Laboratories joined the Task Force at the Task 4F and have thus performed evaluation modelling of STT-1 and STT-1b (McKenna, 1999a and 1999b) and predictive modelling only of STT-2 (McKenna, 1999c). The group has focussed on transport modelling applying the multirate mass transfer model STAMMT-L (Haggerty and Reeves, 1998). The model considers advection, hydrodynamic dispersion and mass transfer caused by diffusion and sorption. Multirate mass transfer may be due to variability in the geometrical, geological and geochemical properties of the fracture, fracture filling material and the rock matrix, e.g. the presence of gouge material, alteration zones, zones with stagnant water. This will give rise to simultaneously acting multirate transfer processes.

The model considers advection-dispersion along a one-dimensional transport pathway where the fracture is conceptualised as having a mobile zone and an immobile zone. The mobile zone contains the flowing water in the fracture whereas the immobile zone refers to the matrix. Mass transfer processes control the transport of solute mass between the two zones. In the TRUE-1 application multirate diffusion and sorption rates were described by a lognormal distribution of mass rate coefficients, implying a structure of layered blocks. The parameters for the mass transfer have been defined in such a way that it is due diffusion and sorption in a matrix.

The model can be used for estimating parameters from experimental data using a least square algorithm to minimise the difference between the observed and modelled data. In the current version it is possible to estimate a total of seven variables describing: the total mass uptake capacity, the mean and standard deviation of the log-normal distribution of diffusion rate coefficients, the retardation factor of the immobile zone, the hydrodynamic dispersion, the dilution factor and the water velocity in the fracture. In

order to perform the parameter estimation a smoothing of the source term was performed using a moving filter with additional manual smoothing.

#### *Tracer test STT-1b*

For the STT-1b three sets of parameter estimations were performed using the experimental breakthrough curves. In the first set six of the parameters were estimated for all of the studied tracers, with the water velocity estimated from the breakthrough of HTO assuming it to act as a fully conservative tracer. In the second set both velocity and dispersivity were estimated from the HTO breakthrough and used for all tracers. The remaining five parameters were estimated from the breakthrough from respective tracer. In the third set, a single rate for mass transfer was assumed eliminating the standard deviation of the mass transfer rate distribution, thus leaving four parameters for the estimation.

The parameter estimations using single rate mass transfer produced fits of similar quality to those using multirate mass transfer with the exception of Rb-86 where no reasonable fit could be obtained with the single rate model. The parameter estimation was to some degree affected by the shape of the source term, which masked off some of the mass transfer processes occurring.

#### *Tracer test STT-2*

Predictive modelling of the STT-2 test was performed with the multirate transfer model. The predictions were based on parameter estimations made for the STT-1 test. The parameters for total mass uptake capacity, mean and standard deviation of the lognormal distribution of diffusion rate coefficients were estimated using fixed values for the dispersion length, retardation factor for the mobile zone, dilution factor and water velocity.

The water velocity and the dilution factor were modified in order to account for the lower pumping rate in STT-2.

### **3.2.9 Nagra/PSI**

The Nagra/PSI modelling team participated in Tasks 4E and 4F (Jakob and Heer, 1998a, 1998b, 1999 and 2000) using a simple model for flow and contaminant transport already successfully applied to the modelling of field migration experiments at Finnsjön and Grimsel. The specific objectives were to explore how information on structural geology could be used in the model, if up-scaling of transport parameters from laboratory experiments is feasible and to obtain information regarding advantages and disadvantages of different competing models, especially concerning the degree of sophistication in the description of the hydrology.

The hydrological part of the model was based on a two-dimensional streamtube concept with the assumption of a homogeneous and isotropic transmissivity field. When evaluating the water flow the fractures were assumed to be an equivalent porous medium with homogeneous flow porosity. An averaged uniform steady-state natural



background flow-field was taken into account. Furthermore, constant injection and pumping rates were assumed.

As a consequence of the high pumping rate in the extraction bore hole the capture zone between the injection and extraction boreholes were considered to be very narrow, in the order of a few centimetres only.

Tracer transport was modelled using a one-dimensional dual porosity approach and using averaged values of the transport parameters constant in space and time. Matrix diffusion was assumed to occur in a limited porous zone adjacent to the fractures with linear sorption to the external surfaces and in the matrix. The character of the sorption surfaces were derived from the geological investigations, considering high porosity fault gouge and lower porosity cataclasite, mylonite and altered rock.

#### *Tracer test STT-1*

For the predictions of STT-1 the model was calibrated by fitting the Uranine breakthrough curve from the PDT-3 tracer test. The shape of the trailing edge of the curve indicated a marked effect of matrix diffusion, which was consistent with former findings of fault gouge material in the vicinity of Feature A. For the blind predictions of the STT-1 test a single family of fractures with a one-sided limited diffusion into fault gouge was assumed. The extent of the diffusion accessible zone was assumed to be 1 mm. Matrix sorption coefficients based on laboratory investigations were rescaled to account for crushing in the batch sorption experiments and to extrapolate to crushed mylonite which was considered to be the material closest to the fault gouge. The values for the pore diffusivities were extrapolated from that for Uranine and using nuclide dependent values for the diffusivity in free water.

A very good fit was obtained for the non-sorbing and weakly sorbing tracers, while the breakthrough time was overpredicted for strongly sorbing tracers such as Rb and Cs.

In the evaluation of the experiments it was found that the assumed value for the thickness of the fault gouge material was too small and needed to be adjusted to 5 mm. The model was first adjusted for the non-sorbing tracer Uranine, then all the other tracers were simulated keeping the nuclide independent parameters constant only the nuclide dependent sorption coefficients were adjusted. However, especially for the more strongly sorbing tracer the early breakthrough found in the experiment could not be simulated. Only when a second flowpath was included could the rising edge be simulated. However, for cesium a significant tracer loss of about 50% had to be assumed.

#### *Tracer test STT-1b*

An update of the model was made for the predictions of the STT-1b test. The update was based on the evaluation of the STT-1 test and a calibration of the Uranine breakthrough obtained in the PDT-4 tracer test. A refinement was made of the geometry for flow and transport considering a second independent family of fractures bounded by a less porous cataclasite, in addition to the family of fractures bounded by fault gouge. Furthermore, the flow width was reduced. The sorption coefficients used for the

predictions were derived from the evaluation of the STT-1 test and differed a maximum by a factor of five from the laboratory data obtained for Äspö diorite.

In the evaluation of the STT-1b test it was observed that for non-sorbing and weakly sorbing tracers a sufficiently good representation could be made considering only a single family of flow paths while for the more sorbing tracers the addition of a second fracture family provided a slightly better fit.

#### *Tracer test STT-2*

Predictions of the STT-2 test were made with the refined geometrical model (two independent fracture families) used for the predictions of STT-1b. The flow field was evaluated from the pumping rate in the extraction hole, the estimated flow rate in the injection bore hole and the natural background flow field as measured on 15<sup>th</sup> December 1998. The values of the flowpath, diffusivity and sorption parameters were derived from the best-fit obtained from inverse modelling of the STT-1 tracer test.

In the subsequent evaluation it was found that the double peak observed for non-sorbing and weakly sorbing tracers in the experimental breakthrough was not represented in the predictions. However, by adjusting the mean water velocities and weights of the two fracture families and fine-tuning of the remaining transport parameters a very good agreement between measured and calculated breakthrough curves could be obtained. The exception was Cs where again a loss of about 30-50% of the tracer had to be taken into account.

## 4 Results

### 4.1 Modelling results

This section gives a brief overview of the modelling results. A more comprehensive compilation of results of STT-1 is given in Ström (1998), of STT-1b in Morosini (1999a), of STT-2 in Morosini (1999b) and in the ICR reports written by the modelling groups.

Most of the modelling groups have used deterministic models, while a few have used stochastic models, consequently some results were given with percentile intervals and some as point estimates. To facilitate the comparison between stochastic and deterministic model approaches the results from the stochastic models are represented as the 50-percentile of the ensemble of predictions. Table 4-1 shows the modelling approach the different groups have used.

**Table 4-1 Model approach used by the different modelling groups.**

<b>Modelling group</b>	<b>Stochastic</b>	<b>Deterministic</b>
CRIEPI		X
JNC/Golder	X	
SKB/KTH-ChE	X	
Posiva/VTT	X	
BMW/BGR		X
SKB/KTH TRUE		X
ANDRA-CEA		X
DOE / Sandia		X
Nagra/PSI		X

The modelling groups have presented their results according to the instructions from the SKB Task Force Secretariat, i.e. breakthrough curves for the performed measurements with listing of  $t_5$  (first breakthrough),  $t_{50}$  (median breakthrough),  $t_{95}$  (tail breakthrough) and mass recovery. The groups using a stochastic approach present their results for the 5-percentile, 50-percentile and the 95-percentile. Not all groups have models that predict drawdown and thus steady state drawdown in the pumping and injection sections is presented only for a selection of groups.

The objectives of the evaluation of STT-1, STT-1b and STT-2 were to increase understanding of transport of sorbing tracers in the studied feature and up to nine different sorbing tracers have been predicted. Figure 4-1, 4-2 and 4-3 shows examples of

the results for the prediction of the moderately sorbing tracer Rubidium-86 for STT-1, STT-1b and STT-2 respectively.

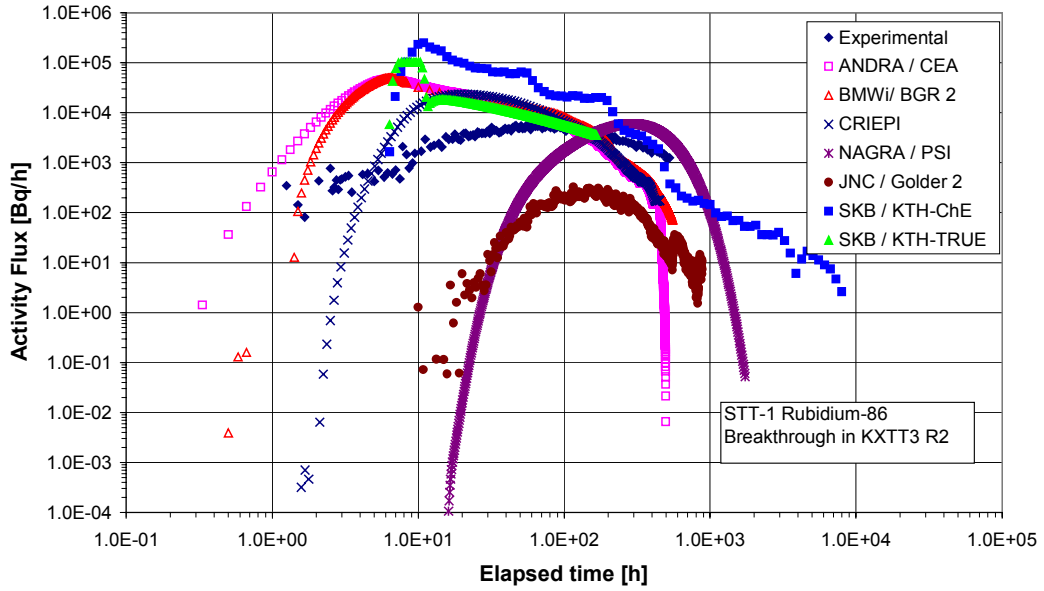


Figure 4-1 Predicted breakthrough for Rubidium-86 from in the STT-1 test.

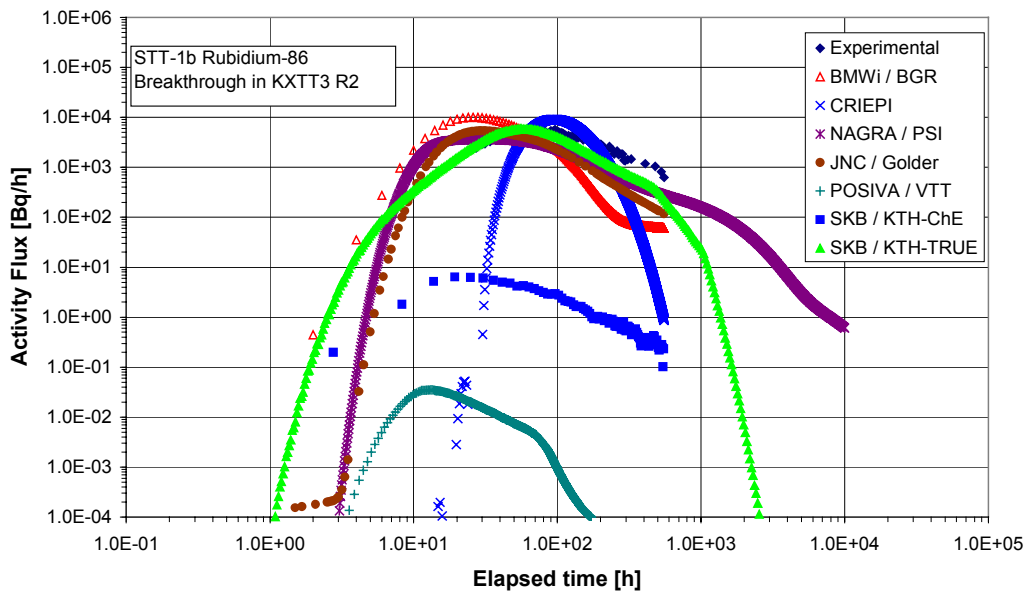


Figure 4-2 Predicted breakthrough for Rubidium-86 in the STT-1b test.

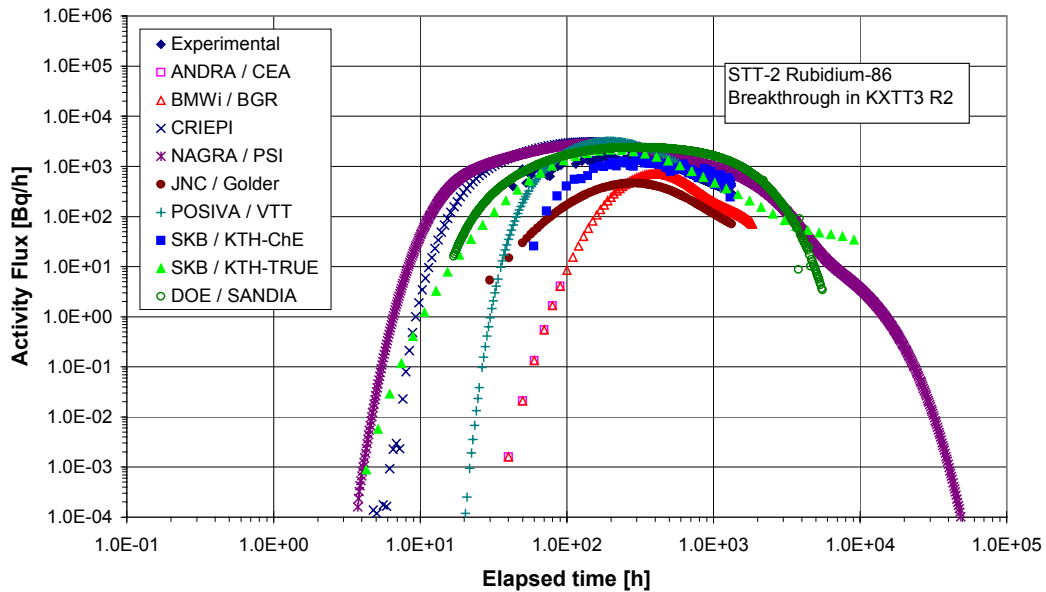


Figure 4-3 Predicted breakthrough for Rubidium-86 in the STT-2 test.

## 4.2 Experimental results

### 4.2.1 Tracer test STT-1

The injection concentrations versus time for the different tracers in STT-1 are shown in logarithmic scale in Figure 4-4. In the borehole section KXTT4 R3 eight tracers were injected, two considered as non-sorbing (Uranine and tritiated water) and six weakly to moderately radioactive sorbing tracers ( $^{22}\text{Na}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$ ,  $^{137}\text{Cs}$ ). There is a sharp increase in concentration during the initial part of the injection, followed by a decline in concentration due to dilution by the flow through the borehole section. The decline is more pronounced for the sorbing radionuclides most likely due to sorption on the borehole walls. After four hours the injection fluid was exchanged with unlabelled water which gives a rapid decrease in concentration. This is followed by an increase in concentration probably due to tracers remaining in a stagnant zone within the injection section. Finally, the concentration declines due to dilution.

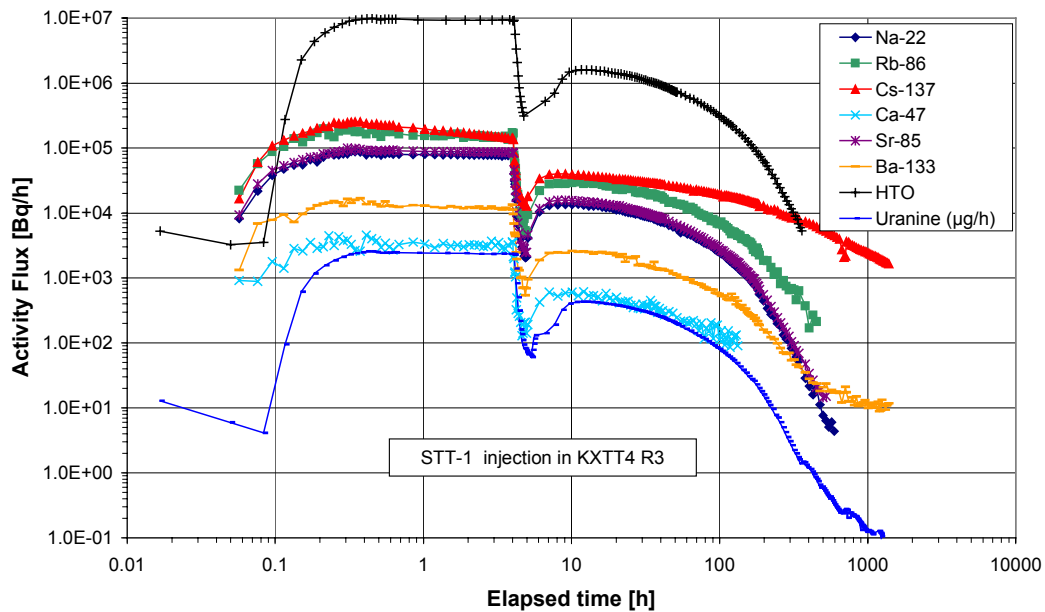


Figure 4-4 Injection flux of tracers in STT-1.

In STT-1 all of the injected tracers were recovered in the pumping section KXTT3 R2. Figure 4-5 shows the breakthrough concentration as a function of time in a logarithmic scale. For Na-22, Sr-85, HTO and Uranine breakthrough occurs at a similar time and the curves also have similar shape. For these tracers there is an indication of a second peak occurring after the primary. The tracers Ba-133, Rb-86 and Cs-137 show a varying degree of retardation in the breakthrough.

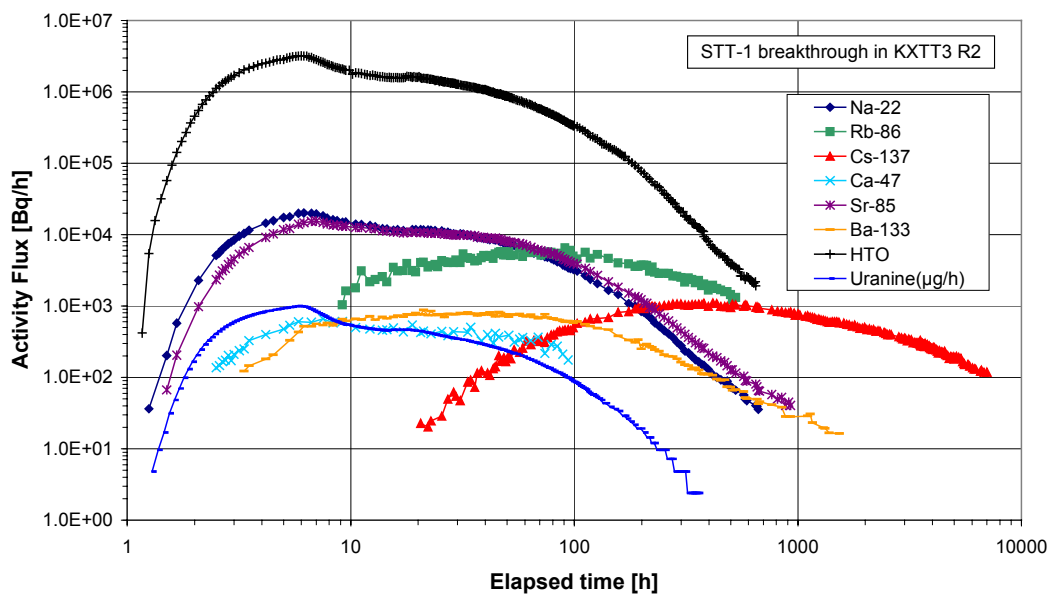


Figure 4-5 Breakthrough curves from STT-1 between KXTT4 R3 and KXTT3 R2.

#### 4.2.2 Tracer test STT-1b

The injection curves in STT-1b have a shape similar to those of STT-1, see Figure 4-6. In the borehole section KXTT1 R2 ten tracers were injected, four non-sorbing (Uranine, HTO,  $^{82}\text{Br}$ ,  $^{131}\text{I}$ ) and six weakly to moderately sorbing ( $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{58}\text{Co}$ ,  $^{99\text{m}}\text{Tc}$ ). As in STT-1 the injection curves show an initial peak with a duration of 4 hours ending with a rapid decline in concentration due to the exchange of water in the injections section. This is followed by an increase in concentration probably due to tracer present in stagnant water in the injection section. The main difference between STT-1 and STT-1b is that in STT-1b there is an additional decline in concentration after about 7 hours, caused by a second exchange in the injection section.

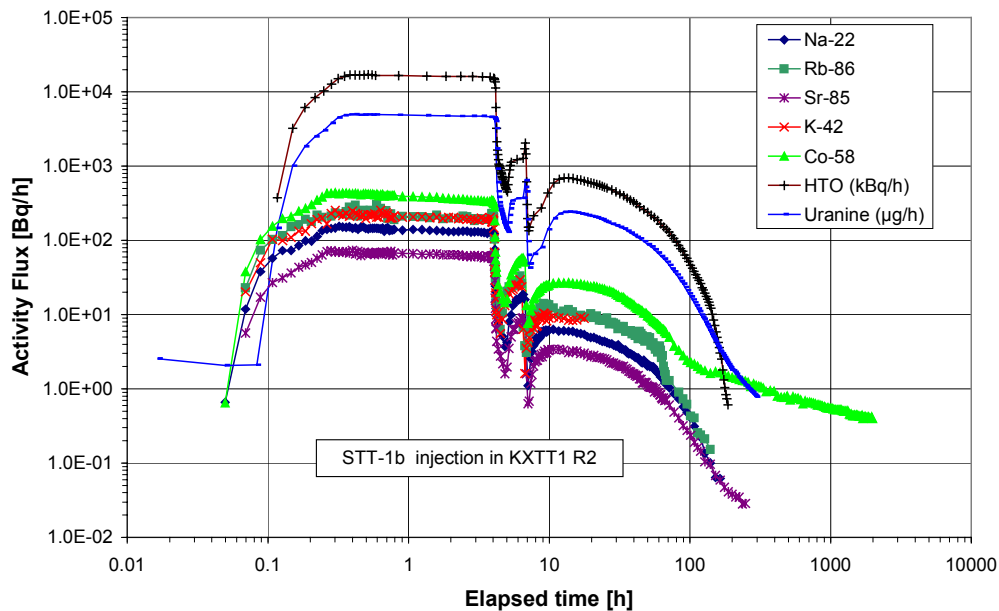


Figure 4-6 Injection flux of tracers in STT-1b.

In the tracer test STT-1b, recovery was obtained for nine of the injected tracers, but not for Tc-99m. Figure 4-7 shows the breakthrough curves as a function of time in a logarithmic scale. Also in STT-1b the curves for HTO, Uranine and Na-22 have a similar shape. A somewhat more pronounced delay of Sr-85 than in STT-1 can be observed. The breakthrough curve of K-42 is rather oscillating and contains only few points. The breakthrough of Rb-86 and Co-58 is considerably delayed.

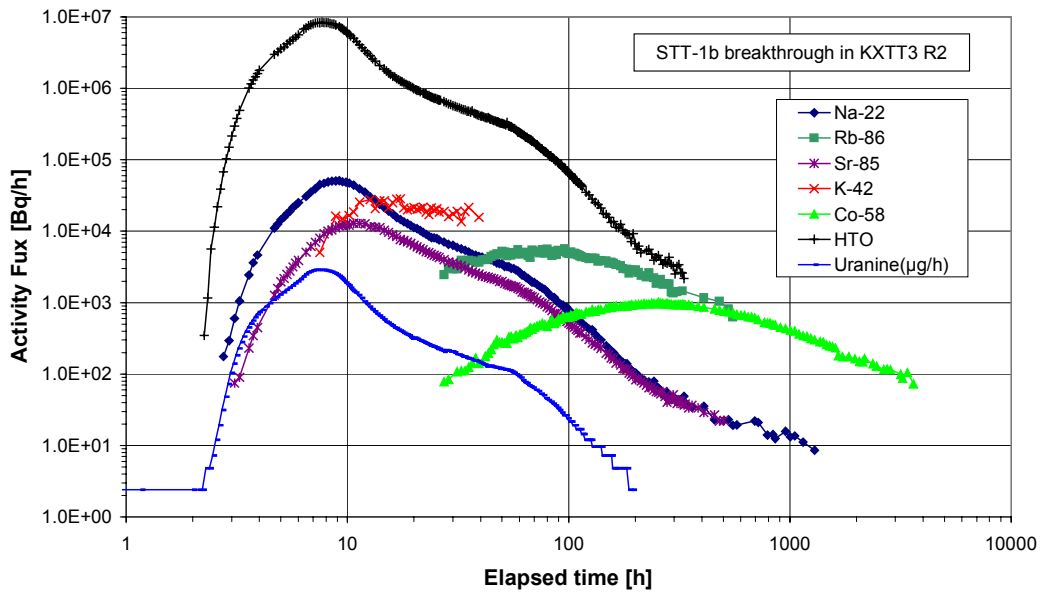


Figure 4-7 Breakthrough curves from STT-1b between KXTT1 R2 and KXTT3 R2.

#### 4.2.3 Tracer test STT-2

The injection procedure in STT-2 was performed in the same way as in STT-1b. The injection curves in STT-2 have a shape similar to those of STT-1b, see Figure 4-8. In the borehole section KXTT4 R3 twelve different tracers were injected, three non-sorbing (Uranine, HTO,  $^{82}\text{Br}$ ) and nine weakly to moderately radioactive sorbing tracers ( $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{99\text{m}}\text{Tc}$ ,  $^{131}\text{Ba}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$  and  $^{137}\text{Cs}$ ).

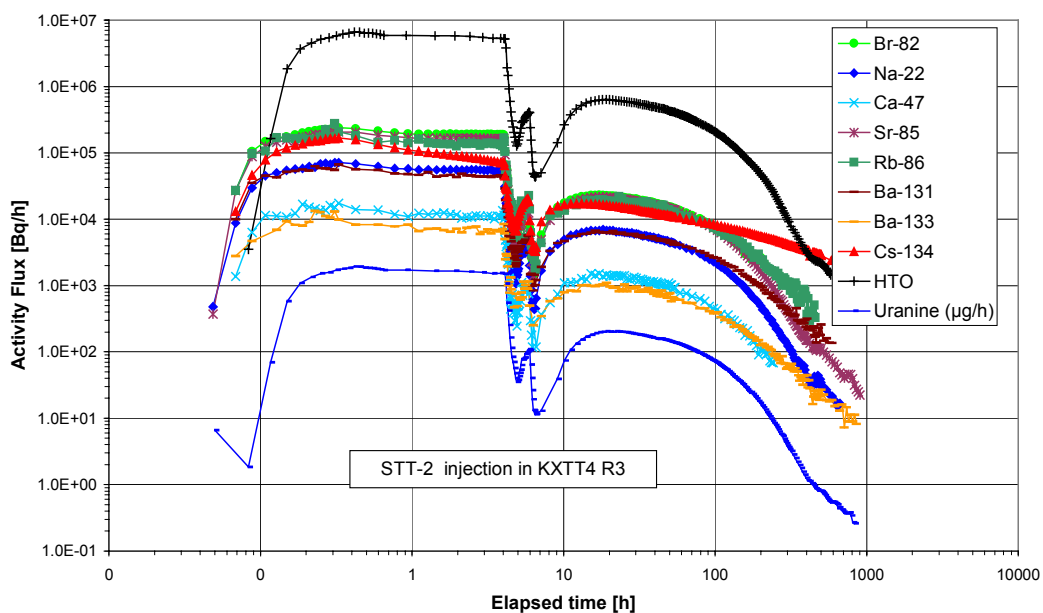


Figure 4-8 Injection flux of tracers in STT-2.



In STT-2 all of the injected tracers except Tc-99m and K-42 were recovered in the pumping section KXTT3 R2. Figure 4-9 shows the breakthrough as a function of time in a logarithmic scale. For HTO, Br-82 and Uranine breakthrough occurs at a similar time and the curves also have a similar shape. For these tracers breakthrough consists of two peaks. The breakthrough for Na-22, Ca-47 and Sr-85 occurs a little bit later but still with a clear indication of two peaks. For Rb-86, Ba-131, Ba-133 and Cs-134 the breakthrough occurs at a later time and no double peak can be identified in the breakthrough curves.

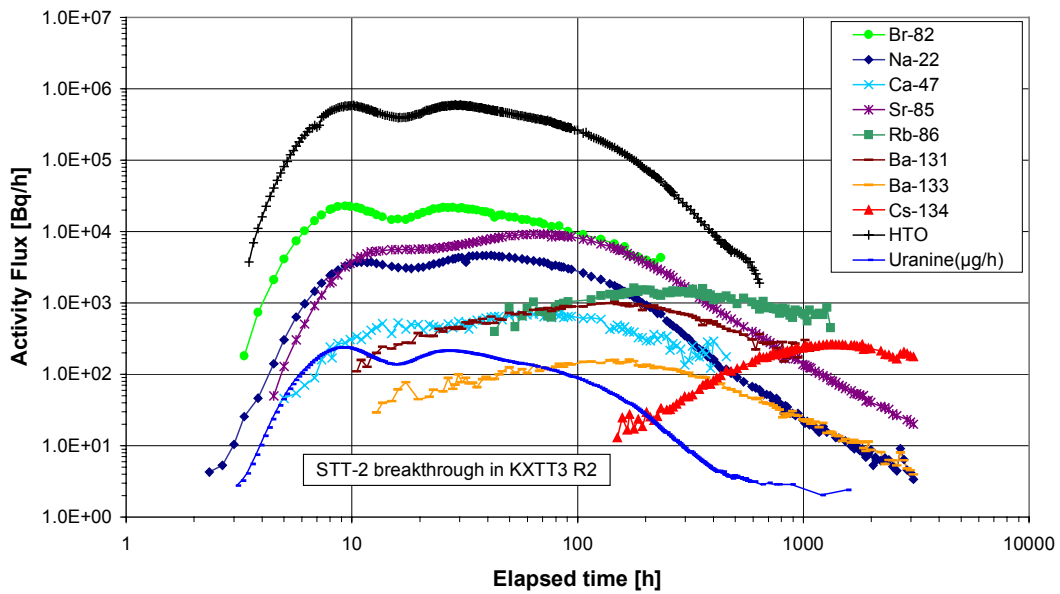


Figure 4-9 Breakthrough curves from STT-2 between KXTT4 R3 and KXTT3 R2.

## 4.3 Comparison of results

### 4.3.1 Performance measures

To facilitate the comparison between the experimental values and the predictions a number of performance measures were defined by the Äspö Task Force. The error in the prediction of a variable  $X$ , originally called measure of accuracy, was defined as:

$$A = \frac{(X_m - X_p)}{X_m} \quad (4-1)$$

where:

$X_m$  is the measured value.

$X_p$  is the point estimate predicted by a deterministic model or the 50-percentile of the ensemble of predictions made with a stochastic model.

With this definition of the accuracy measure a significant underprediction has less effect on the accuracy measure than a significant overprediction. For underpredictions the accuracy measure can never be greater than 1, while for overpredictions large negative values can be obtained.

Furthermore, for each experiment the predicted and the experimental breakthrough time values are plotted against each other in a log-log diagram. The breakthrough time values are represented by the breakthrough times for the recovery of 5, 50 and 95 % of the injected mass. If the predicted breakthrough values correspond to the experimental values they coincide to the diagonal of the log-log diagram. If a value is above the diagonal line the actual model overpredict the breakthrough time and opposite if the value is under the diagonal line the model underpredict the breakthrough time.

To facilitate the performance measurement the predictions are represented by three tracers with different characteristics, one non-sorbing, one weakly sorbing and one moderately sorbing tracer, i.e. Uranine, Strontium-85 and Rubidium-86.

### 4.3.2 Tracer test STT-1

#### *Drawdown*

The modelling groups presenting drawdown values generally made good predictions of the drawdown in the observation wells, but generally underpredicted the drawdown in the pumping well. Note that there was considerable variation in the measured drawdown during the experiment.

**Table 4-2 Predicted and observed drawdown (meters) in STT-1. Median values used for the stochastic models. Pumping in KXTT3.**

MODELS	KXTT1	KXTT2	KXTT4	KA3005A	KXTT3
CRIEPI					5.45
JNC/Golder	2.2	4	1.7	1.4	5.3
Posiva/VTT			2		13
BMWi/BGR				1.2	8.2
<i>Experimental</i>	<i>2.6 - 5</i>	<i>7 - 12</i>	<i>1.1 - 3.5</i>	<i>1.6 - 5</i>	<i>9 - 14</i>

#### *Mass Recovery*

During the experimental time complete recovery was obtained for Uranine from the injection hole, KXTT4, while Sr-85 was almost complete recovered (91%). The moderately sorbing tracer Rb-86 was recovered with 60 %. Table 4-3 shows the predictions made by the modelling groups. A direct comparison is in this case difficult to make, since the percentage recovered was evaluated at different times. For example, JNC/Golder and Nagra/PSI evaluated the recovery after 100 hours which explains the lower predicted recovery. The SKB/KTH-ChE team evaluated the recovery after about 8000 hours, which results in almost full recovery of all tracers.

**Table 4-3 Predicted and observed mass recovery (%) in STT-1. Median values used for the stochastic models.**

MODELS	Uranine	Strontium 85	Rubidium-86
ANDRA / CEA	-	-	-
BMWi / BGR	40	36	36
CRIEPI	99	99	99
NAGRA / PSI	84	83	2
JNC / Golder	75	67	1
POSIVA / VTT	100	100	88
SKB / KTH-ChE	97	99	99
SKB / KTH-TRUE	-	-	-
<b>Experimental</b>	<b>100</b>	<b>91</b>	<b>60</b>
<b>Sampling time</b>	<b>360 h</b>	<b>526 h</b>	<b>526 h</b>

### Breakthrough

For the non-sorbing tracer Uranine most of the models achieve a good prediction of the breakthrough times, see Figure 4-10. However, the JNC/Golder model underpredicts the time for arrival of the 50 and 95% of the injected mass.

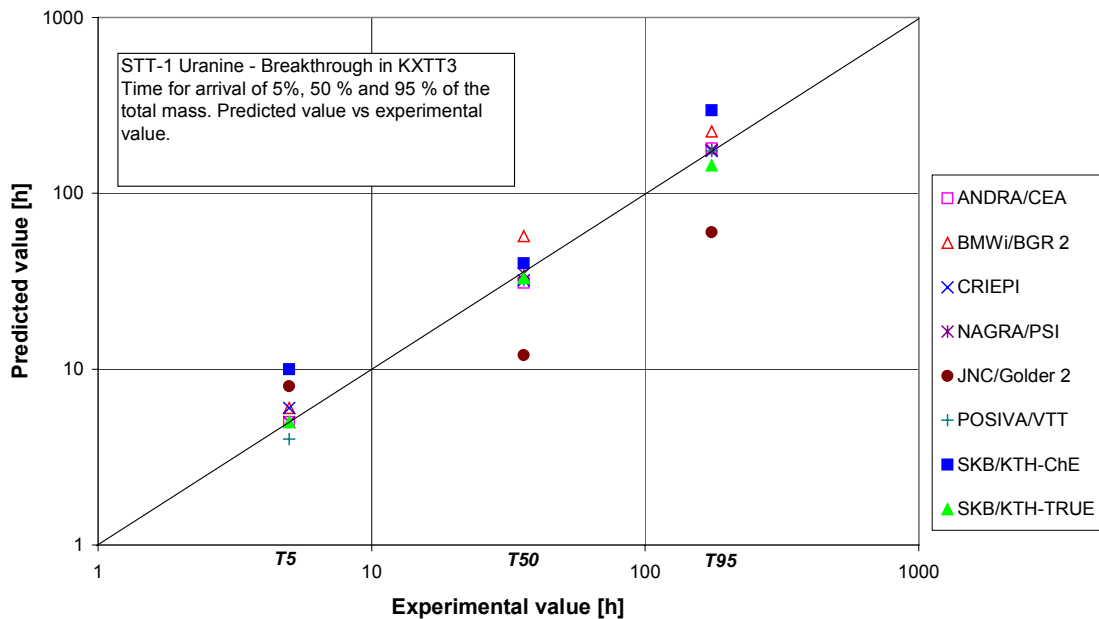


Figure 4-10 Predictions of breakthrough time for Uranine in STT-1.

Since the recovery of Strontium-85 was less than 95%, performance measures are only made for the time for arrival of 5 and 50% of the injected mass, see Figure 4-11. The breakthrough time for Sr-85 was generally underpredicted for all models except for the SKB/KTH-ChE model, which slightly overpredicted the time for arrival of 5% of the injected mass.

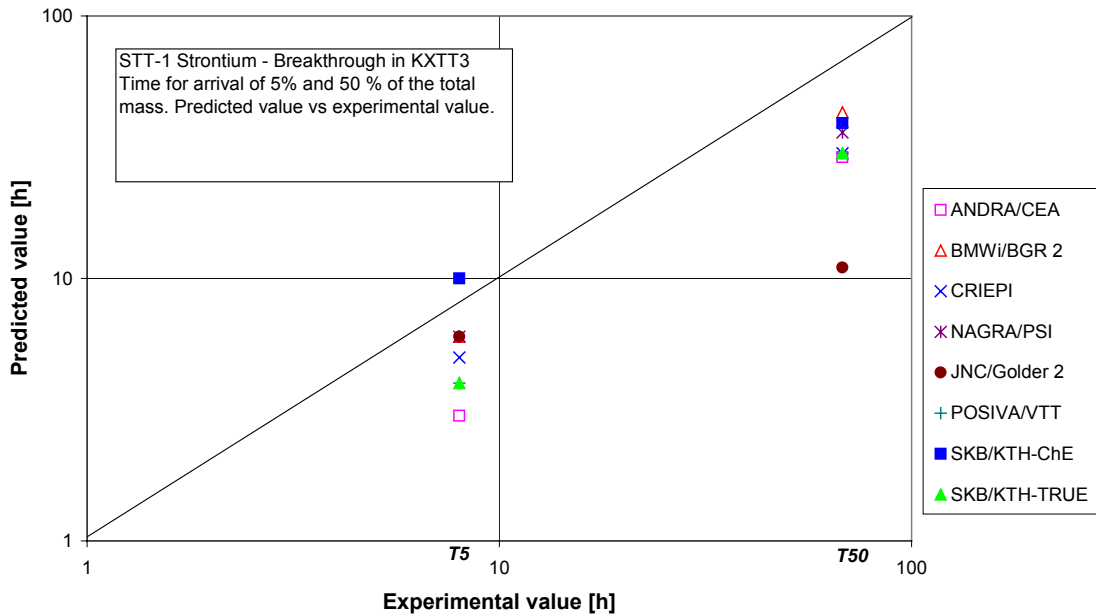


Figure 4-11 Predictions of breakthrough time for Strontium in STT-1.

The breakthrough time ( $t_5$  and  $t_{50}$ ) for Rubidium-86 was significantly underpredicted for most of the models (Figure 4-12). However, for the arrival of 5% of the injected mass JNC/Golder and NAGRA/PSI showed an overprediction, while the  $t_{50}$ -value for NAGRA/PSI was very close to the experimental value.

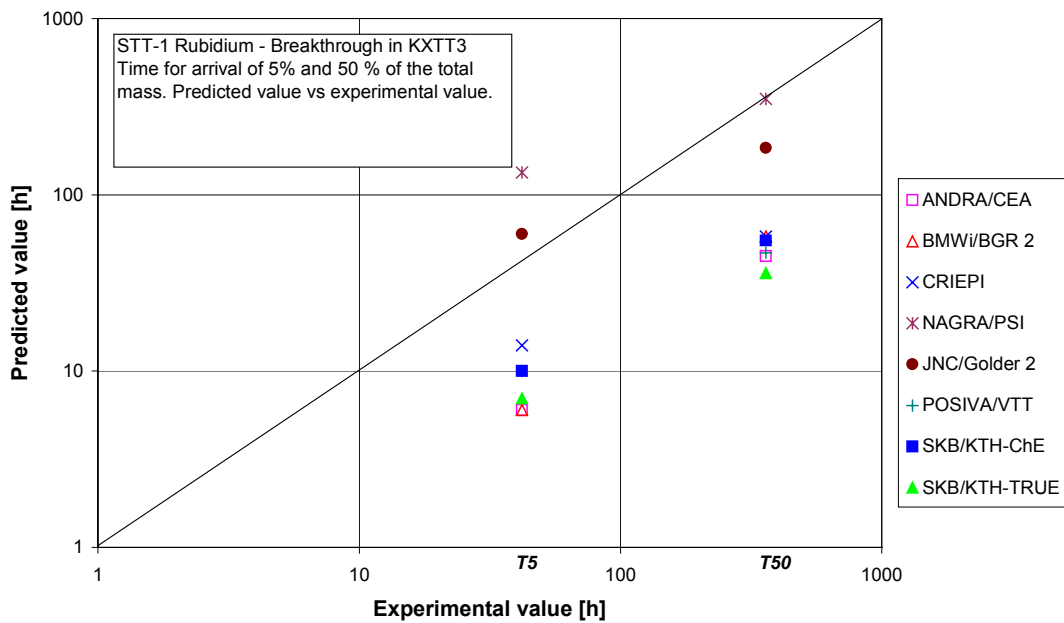


Figure 4-12 Predictions of breakthrough time for Rubidium in STT-1.

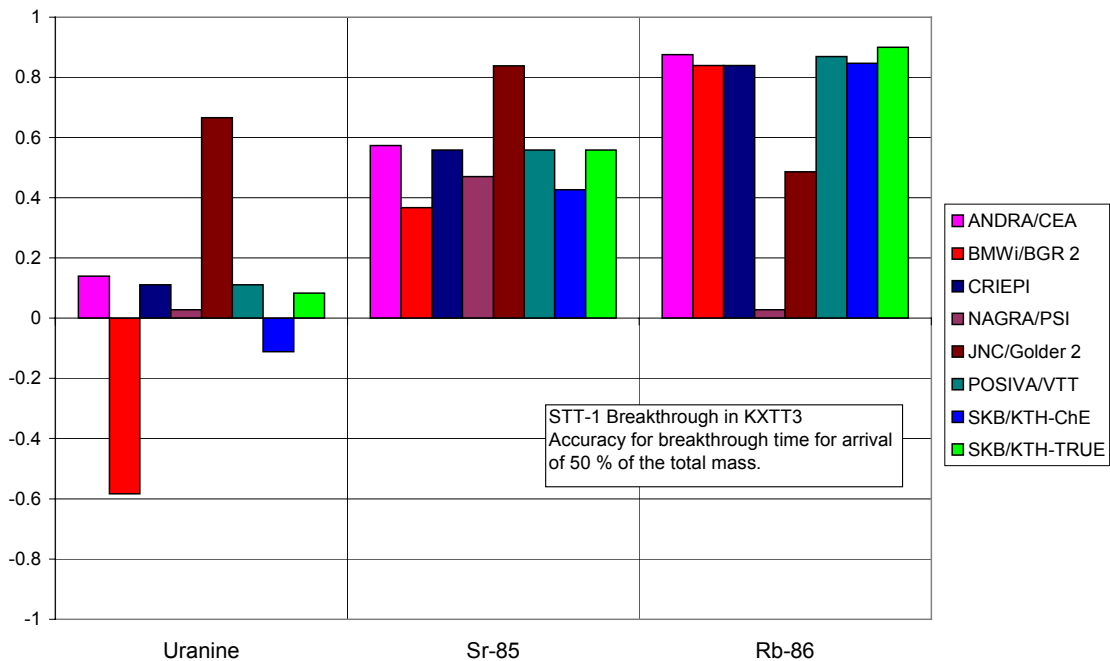


Figure 4-13 Accuracy for predicted time for arrival of 50% of the injected mass for STT-1.

### 4.3.3 Tracer test STT-1b

#### Drawdown

The modelling groups presenting drawdown values generally made good predictions of the drawdown in the observation wells, but with a slight underprediction of the drawdown in the pumping well. Note that there was considerable variation in the measured drawdown during the experiment.

Table 4-4 Predicted and observed drawdown (meters) in STT-1b. Median values used for the stochastic models.

MODELS	KXTT1	KXTT2	KXTT4	KA3005A	KXTT3
CRIEPI					5.45
JNC/Golder	4.6	10.8	5.9	4.2	12
SKB/KTH-ChE	3.4	3.0	4.0	2.4	11.4
Posiva/VTT			2		13
BMWi/BGR	1.47	2.76	0.41		10.84
<i>Experimental</i>	<i>4</i>	<i>12</i>	<i>2.4</i>	<i>2.3</i>	<i>15</i>

#### Mass Recovery

During the experimental time complete recovery was obtained for Uranine from the injection hole, KXTT4, while the moderately sorbing tracer Rubidium-86 was almost completely recovered (93%). The weakly sorbing tracer Strontium-85 was recovered with

81 %. The predictions of recovery were in this case made for the same time as the experimental sampling time. As shown in Table 4-5 most of the modelling groups predicted almost full recovery of Uranine. For Sr-85 all the modelling groups overpredicted the mass recovery except BMWi/BGR which was very close to the experimental value. For Rb-86 most groups underpredicted the mass recovery, only CRIEPI and POSIVA/VTT made a slight overprediction.

**Table 4-5 Predicted and observed mass recovery (%) at  $T_{100}$  in STT-1b. Median values used for the stochastic models.**

MODELS	Uranine	Strontium-85	Rubidium-86
BMWi / BGR	86	82	69
CRIEPI	100	100	100
NAGRA / PSI	97	100	71
JNC / Golder	98	97	81
POSIVA / VTT	100	100	100
SKB / KTH-Che	98	99	66
SKB / TRUE	106	100	86
<i>Experimental</i>	<i>100</i>	<i>81</i>	<i>93</i>
<i><math>T_{100}</math></i>	<i>195</i>	<i>505</i>	<i>553</i>

### Breakthrough

For the non-sorbing tracer Uranine most of the models slightly overpredicted the breakthrough times except for the JNC/Golder and CRIEPI model which achieve a good accuracy, see Figure 4-14. POSIVA/VTT slightly underpredict the breakthrough times.

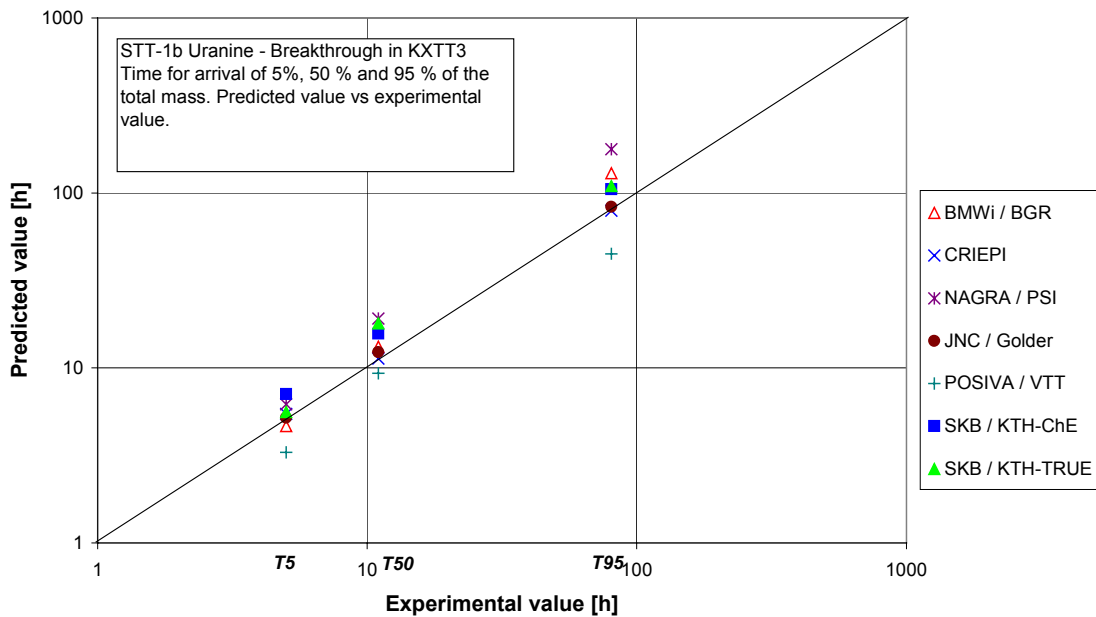


Figure 4-14 Predictions of breakthrough time for Uranine in STT-1b.

The time for arrival of 5 and 50% of the injected mass for Strontium-85 is generally underpredicted (Figure 4-15). However, the NAGRA/PSI model prediction is close to the experimental. The recovery of Sr-85 was less than 95% of the injected mass.

The breakthrough time ( $t_5$  and  $t_{50}$ ) for Rubidium-86 was underpredicted in a varying degree for most of the models except for CRIEPI which achieve a good accuracy with only a slight overprediction, see Figure 4-16.

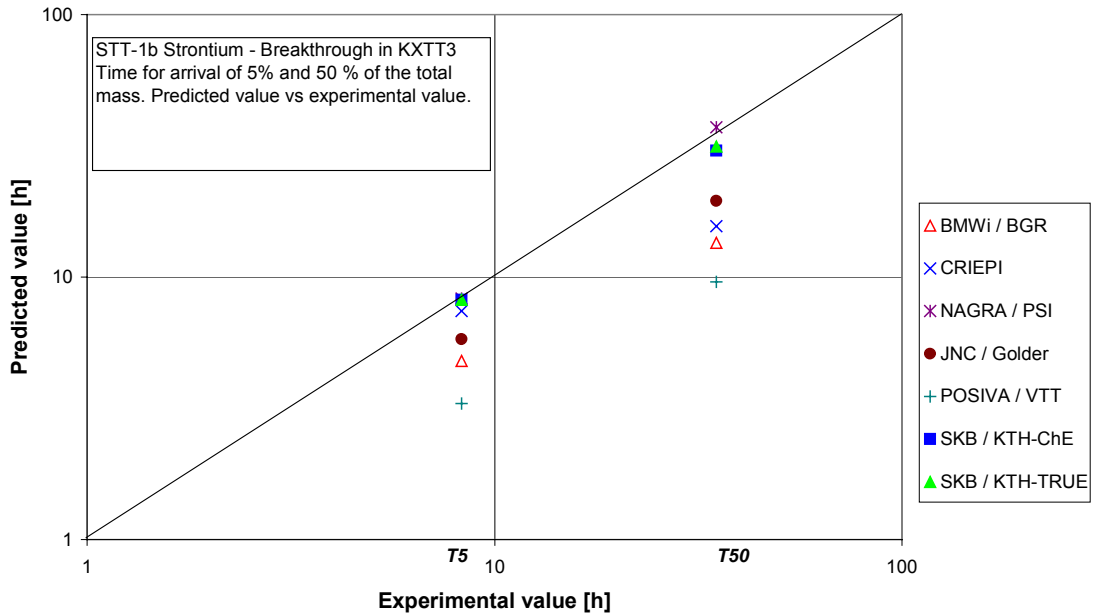


Figure 4-15 Predictions of breakthrough time Strontium in STT-1b.

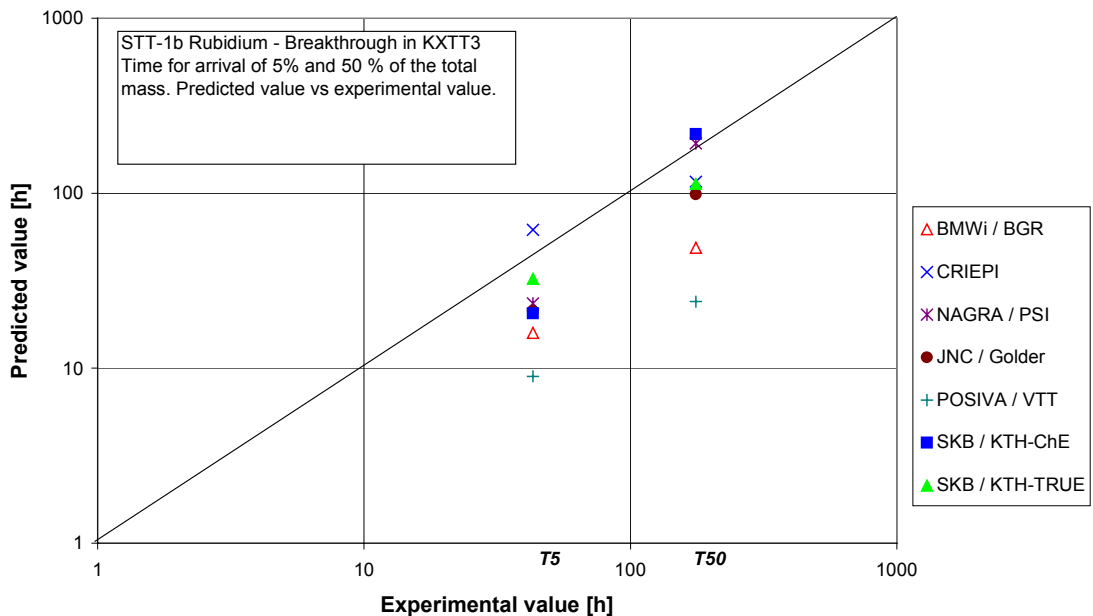


Figure 4-16 Predictions of breakthrough time for Rubidium in STT-1b.

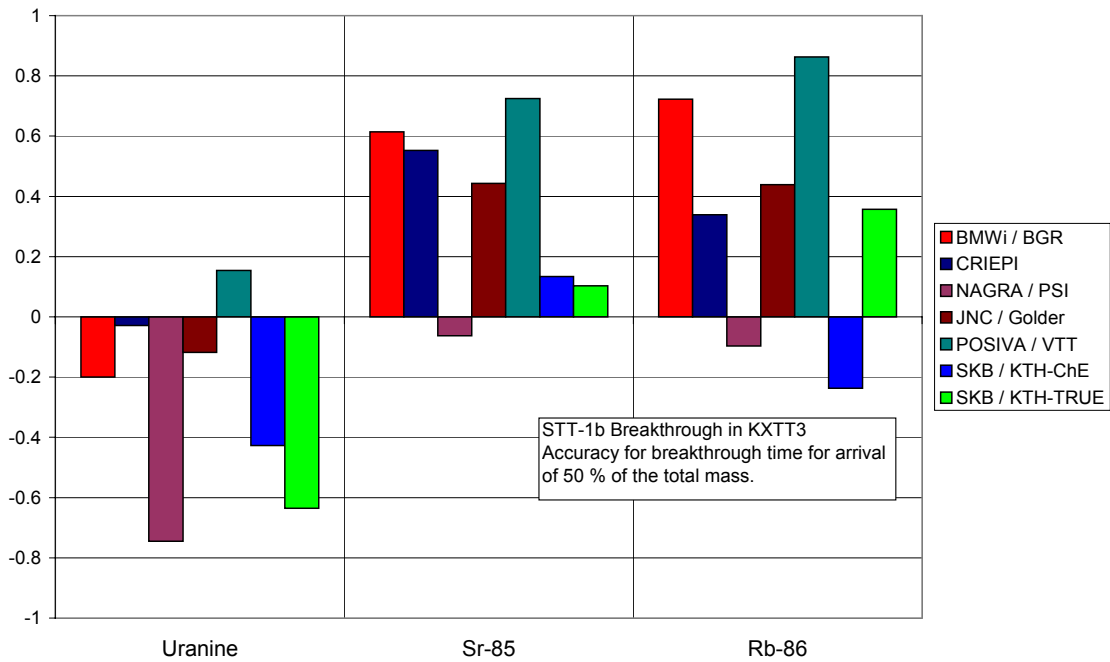


Figure 4-17 Accuracy for predicted time for arrival of 50% of the injected mass for STT-1b.

#### 4.3.4 Tracer test STT-2

##### Drawdown

The modelling groups presenting drawdown values generally made good predictions of the drawdown in the observation wells (KXTT1 and KXTT4), but generally underpredicted the drawdown in KXTT2. The drawdown in the pumping well (KXTT3) was slightly underestimated. Note that there was considerable variation in the measured drawdown during the experiment.

**Table 4-6 Predicted and observed drawdown (meters) in STT-2. Median values used for the stochastic models.**

MODELS	KXTT1	KXTT2	KXTT4	KA3005A	KXTT3
BMWi / BGR	0.74	1.38	0.20		5.42
CRIEPI	1.77	1.16	1.83	0.56	2.73
JNC / Golder	0.14	2.4	0.8	0.29	3.1
SKB / KTH-ChE	1.7	1.5	2.0	1.2	5.7
<b>Experimental</b>	<b>2.0</b>	<b>5.4</b>	<b>1.3</b>	<b>1.2</b>	<b>6.7</b>



## Mass Recovery

Almost complete recovery for Uranine (96 %) and a recovery of 79 % for strontium was obtained during the STT-2 experimental time, Table 4-7. For rubidium the recovery was 49 %. All the modelling groups predicted full or high recovery of both Uranine and strontium. For strontium most of the modelling groups overpredicted the mass recovery. For rubidium the results from the different modelling groups showed varying results with both over- and underpredictions, but mainly overpredictions.

**Table 4-7 Predicted and observed mass recovery (%) at  $T_{100}$  in STT-2. Median values used for the stochastic models.**

MODELS	Uranine	Strontium 85	Rubidium-86
ANDRA / CEA	100	96	
BMWi / BGR	100	93	14
CRIEPI	100	96	61
DOE / SANDIA	99	98	70
JNC / Golder	100	90	8
NAGRA / PSI	100	100	71
POSIVA / VTT	99	95	70
SKB / KTH-ChE	83	80	26
SKB / KTH-TRUE		100	67
<b>Experimental</b>	<b>96</b>	<b>79</b>	<b>49</b>
<b><math>T_{100}</math></b>	<b>885 h</b>	<b>3078 h</b>	<b>1322 h</b>

## Breakthrough

For the time arrival of 5 and 50% of the injected mass for Uranine most of the models achieved a good prediction except for BMWi/BGR that makes a slight overprediction, see Figure 4-18. However, for all models the final part of the breakthrough time ( $t_{95}$ ) is overpredicted.

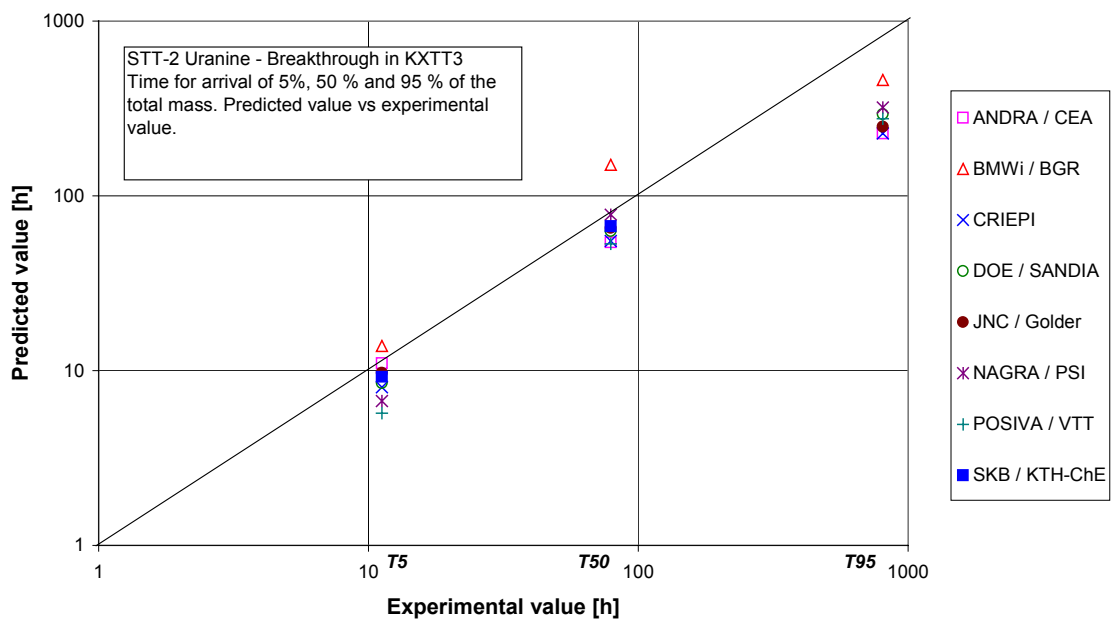


Figure 4-18 Predictions of breakthrough time for Uranine in STT-2.

The breakthrough time ( $t_5$  and  $t_{50}$ ) for Strontium-85 is underpredicted for most of the models (see Figure 4-19). The recovery of Sr-85 was less than the 95% of the injected mass. For the arrival of 5% of the injected mass JNC/Golder, SKB/KTH-ChE and BMWi/BGR showed an overprediction, see Figure 4-20. The other models underpredict the breakthrough time ( $t_5$ ) except for DOE/Sandia which achieved a good accuracy.

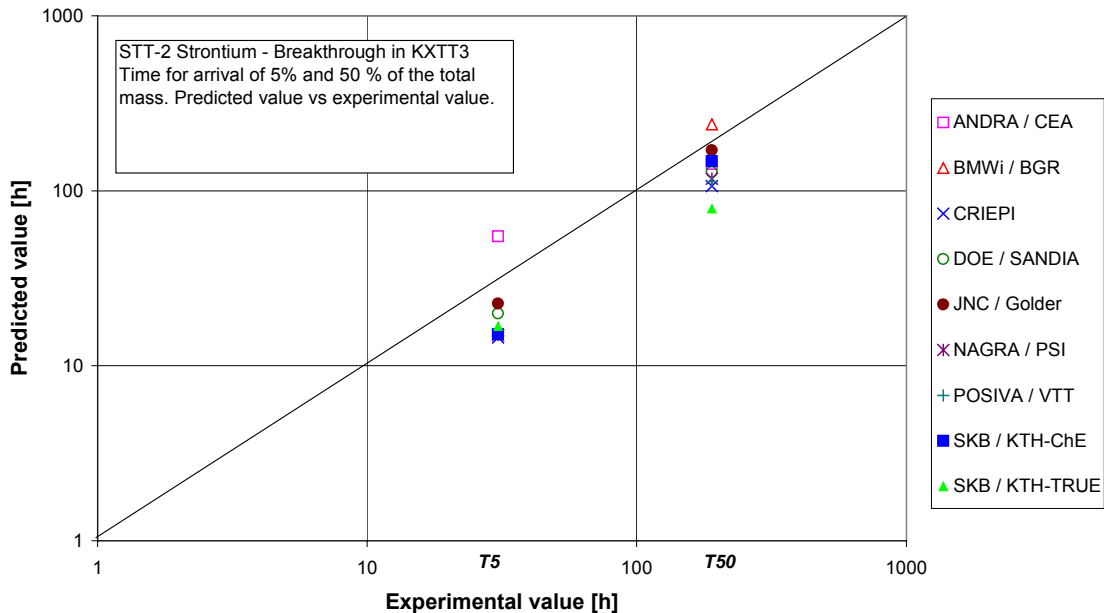


Figure 4-19 Predictions of breakthrough time for Strontium in STT-2.

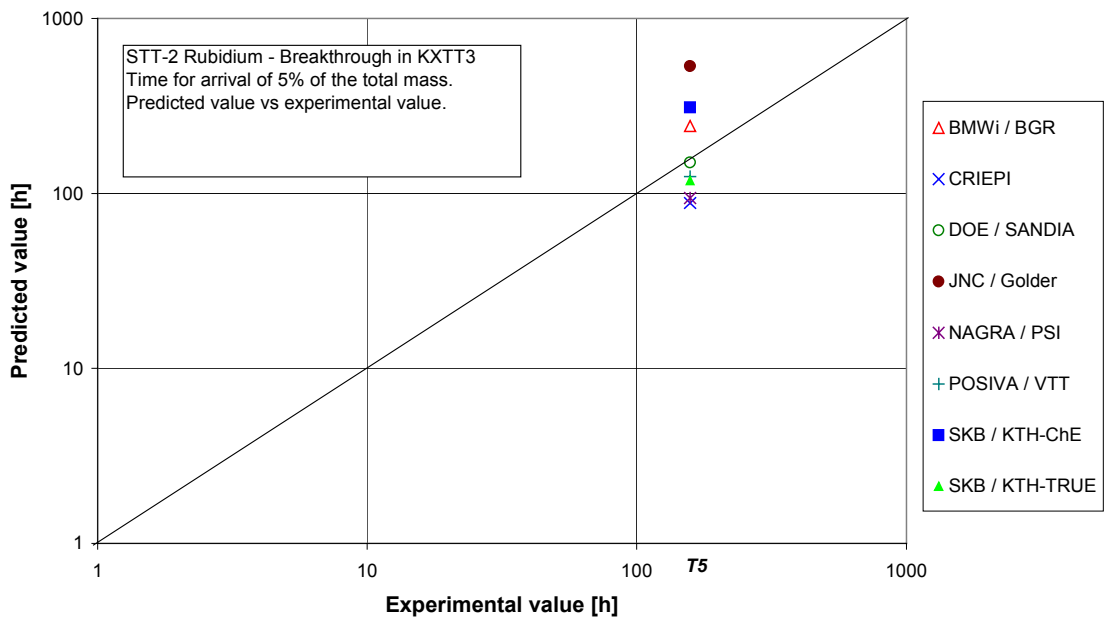


Figure 4-20 Predictions of breakthrough time for Rubidium in STT-2.

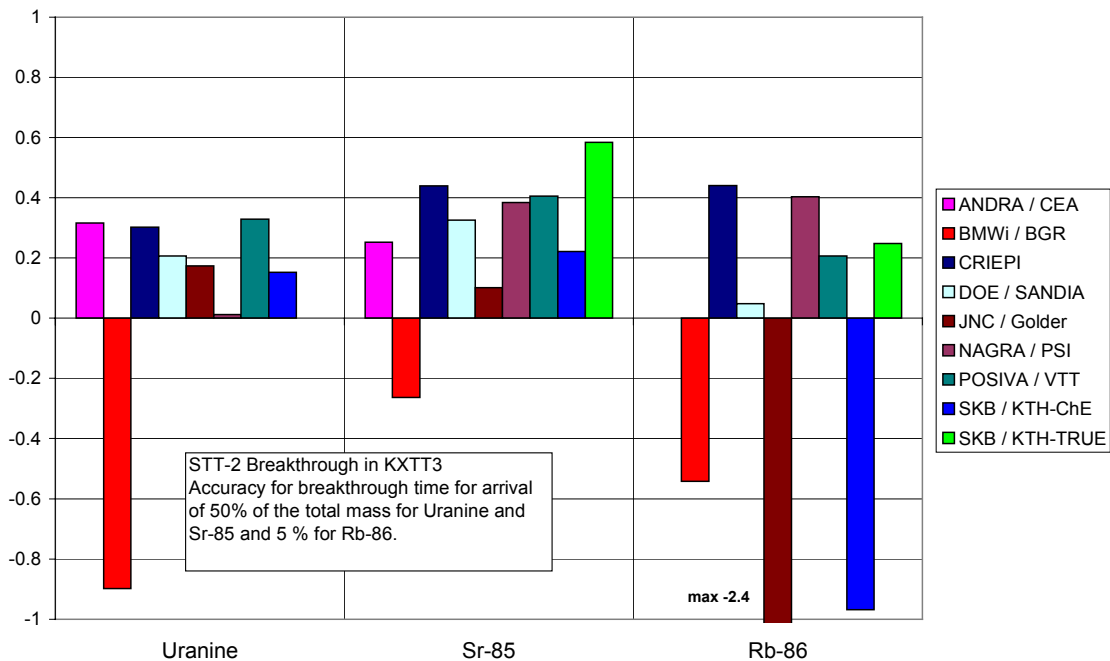


Figure 4-21 Accuracy for predicted time for arrival of 50% of the injected mass for Uranine and Sr-85 and 5% for Rb-86 in STT-2.

## 4.4 Deconvolution as an evaluation approach

### 4.4.1 Introduction

Convolution and deconvolution techniques are used in signal processing and in other areas to analyse linear systems where the output function is given by an input function and a unit response function. For evaluation of tracer transport convolution can be used to obtain a breakthrough curve for a given injection curve when the unit response function is known, see Figure 4-22. Convolution is often used in mathematical modelling of solute transport. In this case a single unit response function for a system is calculated and then used to derive breakthrough curves for arbitrary input functions.

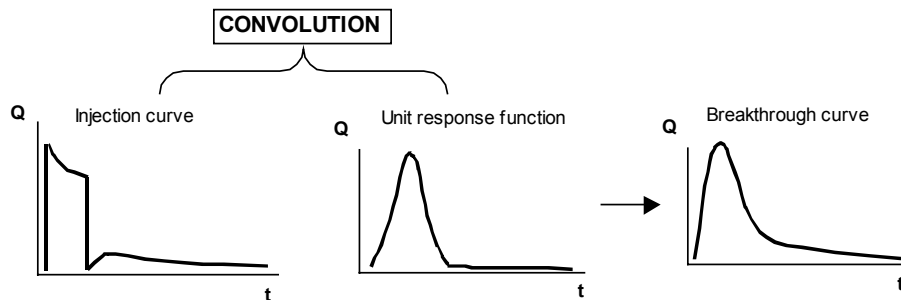


Figure 4-22 Principle of convolution.

The inverse of convolution is called deconvolution and can be used to find the unit response function from the injection curve and the breakthrough curve. The unit response function describes how the breakthrough curve would look like if the injection curve was a Dirac delta function, i.e. a pulse with unit mass and zero duration. In Figure 4-23 the deconvolution principle is described schematically.

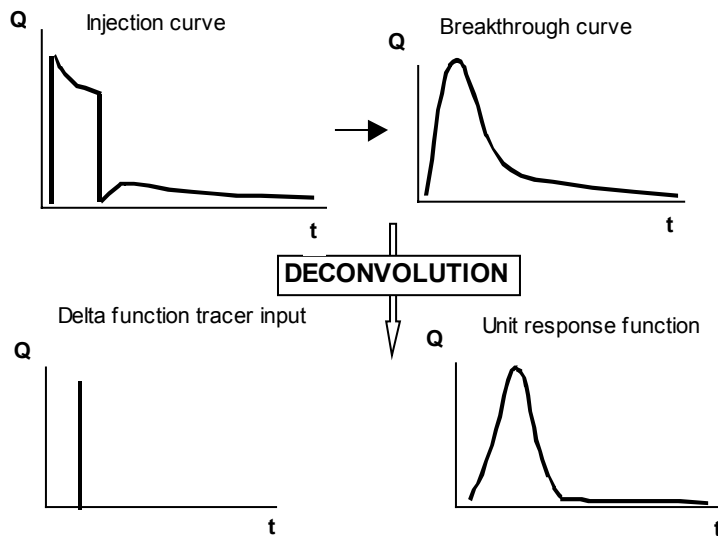


Figure 4-23 Principle of deconvolution.

The unit response function describes the characteristic features of the particular flow and transport problem determined by the transport mechanisms along the flowpaths.

For the Task 4E and 4F many of the models derive unit response functions as a part of the transport calculations, or give such output functions. In this section comparison is made between deconvoluted unit response functions from the STT-2 experiment and predicted output functions based on Dirac pulse injections.

#### 4.4.2 Evaluation

Deconvolution has been performed of the experimental results of the tracer tests STT-1 and STT-1b (Elert and Svensson, 1999) and STT-2 (Elert and Svensson, 2000). Unit response functions have been derived from the experimental injection and breakthrough curves using the Toeplitz method (Tsang et al., 1991). Since deconvolution is an illconditioned problem, were small experimental errors give rise to oscillations, various types of filtering has been applied. However, oscillation in the tails is still apparent in many cases.

In Figure 4-24 the unit response functions the non-sorbing tracer Uranine, the weakly sorbing tracer Strontium-85 and the moderately sorbing tracer Rubidium-86 from STT-2 have been compiled. The double peak is apparent in the unit response functions of Uranine and an indication of a double peak is also apparent for Sr-85. There are a number of oscillations in the unit response function of Rb-86, making identification of a double peak difficult.

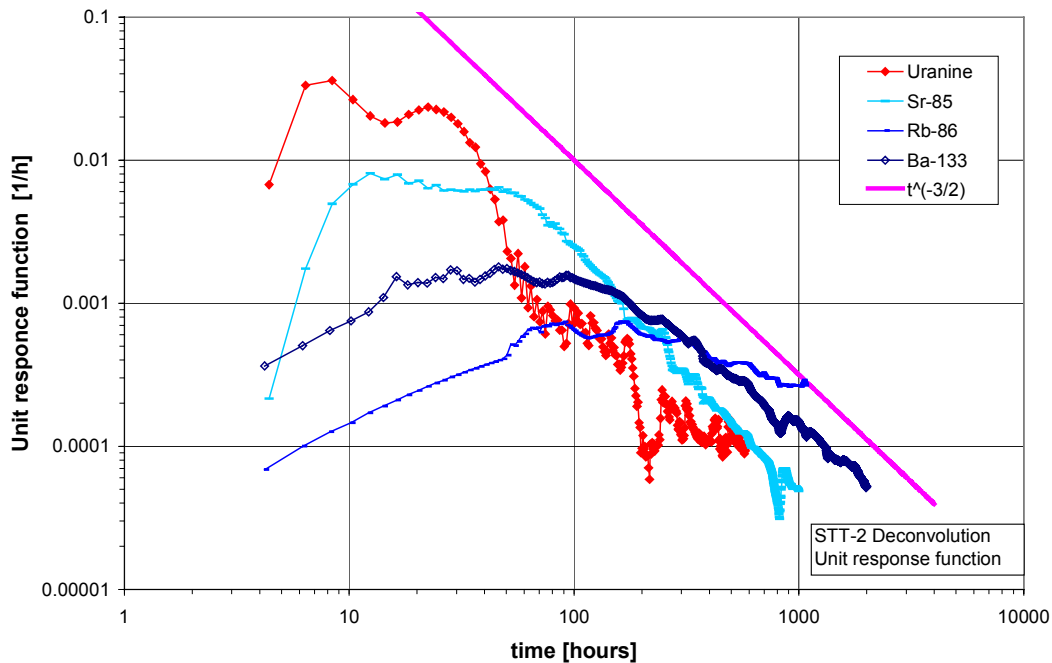


Figure 4-24 Unit response functions for tracers in STT-2.

If matrix diffusion and sorption is the main retardation process, the tail will have a slope of  $-3/2$  in a log-log scale. The deconvoluted unit response curve of Uranine has a slope that is roughly  $-3/2$ , while the slope for Sr-85 is slightly steeper. For Rb-86 the slope is cut-off before any characteristic slope has developed.

Figures 4-25 to 4-27 show a comparison between the predicted cumulative breakthrough curves obtained from the Dirac pulse modelling and the cumulative unit response curve obtained from deconvolution of the experimental results.

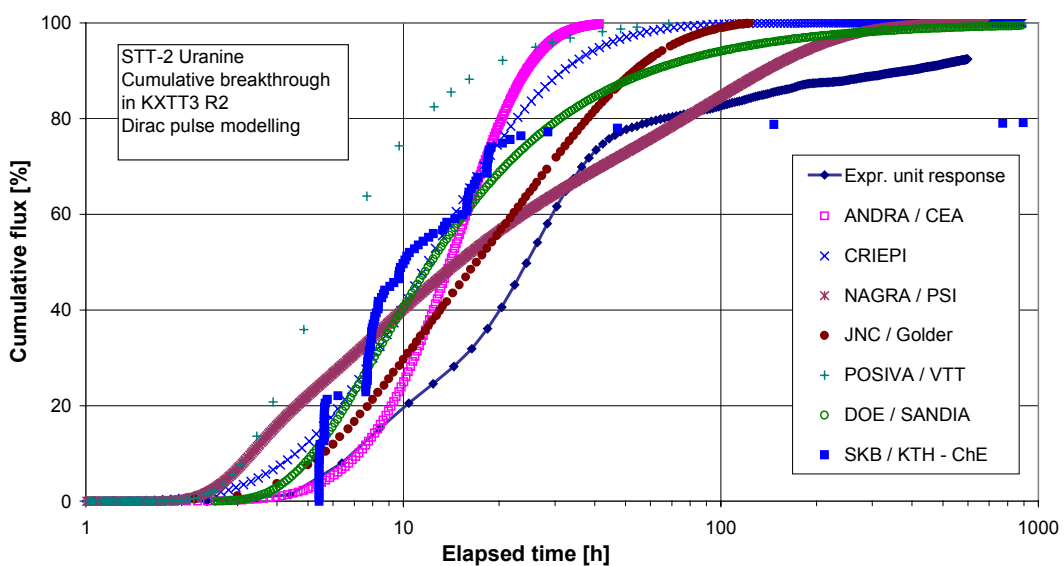


Figure 4-25 Predicted cumulative breakthrough curves based on Dirac pulse modelling for Uranine in the STT-2 experiment.

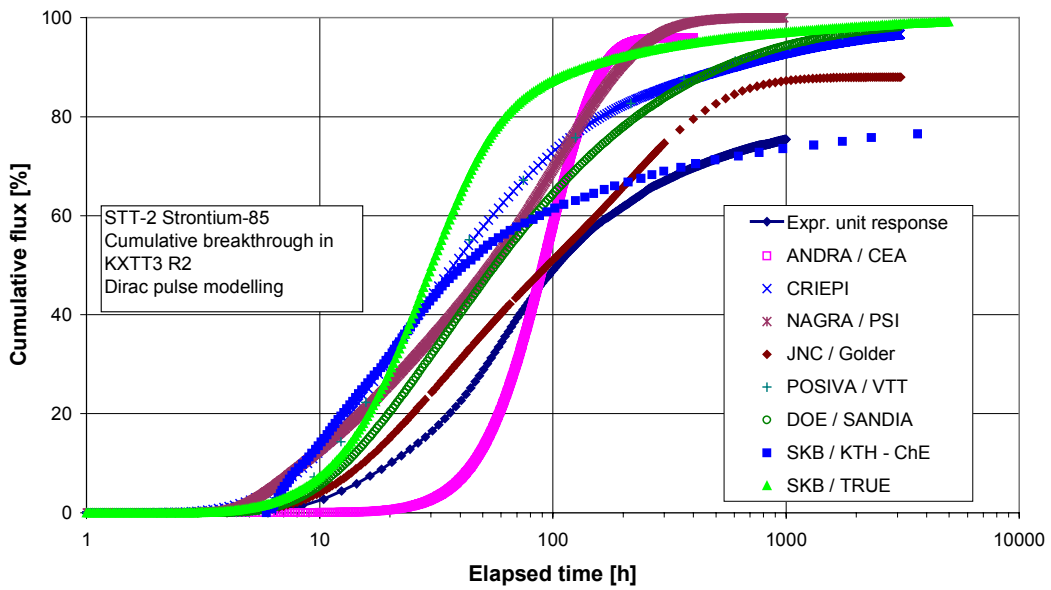


Figure 4-26 Predicted cumulative breakthrough curves based on Dirac pulse modelling for Strontium-85 in the STT-2 experiment.

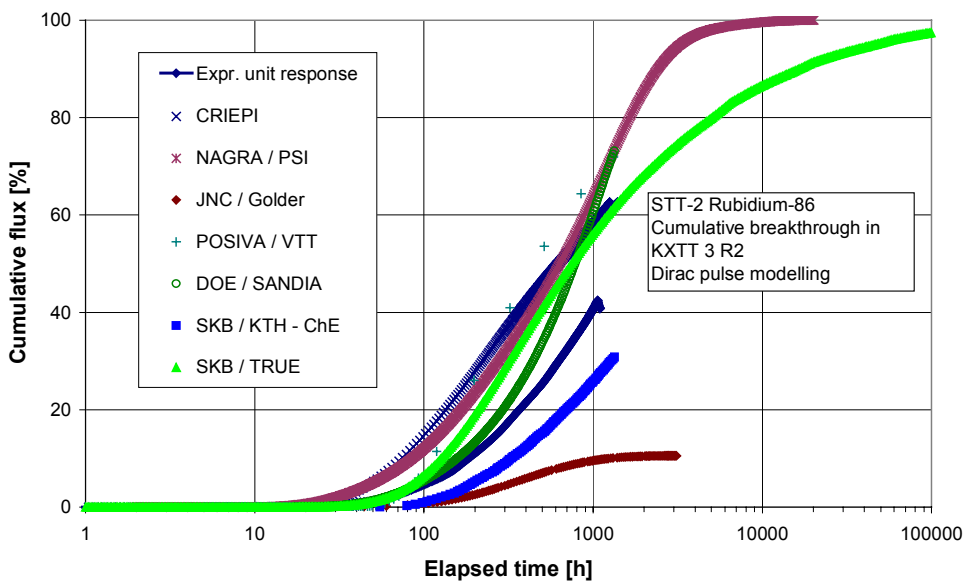


Figure 4-27 Predicted cumulative breakthrough curves based on Dirac pulse modelling for Rubidium-86 in the STT-2 experiment.

## **5 Discussion**

### **5.1 Model geometry and structural model**

The modelling groups have basically retained the model geometry and structural model used in the predictions of the non-sorbing tracer experiments in Task 4C and 4D. This model is based on the available structural-hydraulic model of the TRUE-1 site (Winberg, 1996). The majority of groups have treated Feature A as an isolated single feature, with some exceptions. The JNC/Golder team that used a discrete fracture model including three deterministic features and stochastic background fractures in a considerably larger domain. The SKB/KTH-ChE team included also channels in fractures in the surrounding rock, the nearby Feature B and the tunnel. Feature B was also included in the model of the BMWi/BGR, but was found to have negligible influence on the flow in Feature A.

The more detailed description of Feature A given in Winberg et al. (1998) giving information on geological, structural and hydraulic characteristics of Feature A came at a late stage in the task and has to some extent been incorporated into the models. This has been done by including different types of geological materials (gouge material, altered rock, cataclasite, etc.) in the vicinity of the fracture into which tracers can diffuse. The need to include matrix diffusion has led to model development in several cases. CRIEPI has extended their model to three dimension including a matrix part extending perpendicular to Feature A. BMWi/BGR started with a similar approach, but found it too computationally demanding and therefore changed to a 2D fracture model with 1D matrix element attached perpendicular to the fracture plane to represent the matrix.

### **5.2 Modelling of processes**

The focus of Task 4E and 4F has been on the transport processes especially those of importance for sorbing tracers. Generally, less effort has been put on the hydrological modelling, a subject extensively covered in the previous Tasks 4C and 4D. The water flow is modelled as Darcy flow determined by head gradients and transmissivity or hydraulic conductivity. However, there are considerable differences between the modelling groups in the degree of detail in the hydrological modelling and in the way it is connected to the transport modelling.

### *Hydrological modelling*

A homogeneous transmissivity field in Feature A was assumed in the modelling performed by the Nagra/PSI team and the ANDRA/CEA team. The DOE/Sandia team did not perform any hydrological modelling, instead they derived a water velocity from parameter estimation on previous tracer experiments. The Posiva/VTT team did not perform any hydrological modelling in Task 4F, but derived the water velocity from previously performed tracer tests.

The modelling groups investigating heterogeneous flow in the preceding tasks have based their modelling on previous work, in some cases making modifications or additional calibration. The JNC/Golder team has for Tasks 4E and 4F included a heterogeneous transmissivity field in Feature A, studying different models for generating the field and also comparing it with a homogeneous field. The ANDRA/CEA team has also studied the effect of various methods to generate a heterogeneous transmissivity field in Task 4F. The SKB/KTH-TRUE team used a stochastic continuum model for the flow calculations that included a spatially variable fracture aperture, which was believed to reduce the need for calibration of tracer travel time. The CRIEPI and Posiva/VTT teams have retained their methods for generating the heterogeneous transmissivity field and the BMWi/BGR team uses the same method as in previous tasks of generating a heterogeneous transmissivity field using an iterative deterministic technique. Also the SKB/KTH-ChE team retained their method for generating the conductances in their channel network model.

### *Coupling hydrology to transport*

The coupling between hydrology and transport differs between the different modelling teams. The CRIEPI and BMWi/BGR teams have performed transport calculations using the advection-dispersion equation in the two-dimensional flow field obtained from the hydrological calculations. The SKB/KTH-TRUE and Posiva/VTT teams have used particle tracking to determine residence time distributions of non-sorbing tracers which is used as input in the transport models for sorbing tracers. The JNC/Golder team has used a pathway analysis to determine tracer flowpaths. The SKB/KTH-ChE team used a particle following technique for non-sorbing as well as sorbing tracers. The ANDRA/CEA, Nagra/PSI, DOE/Sandia and Posiva/VTT (Task 4F) used calculated water velocities and in the case of Nagra/PSI and Posiva/VTT also flowpath dimensions.

### *Transport modelling*

Advection is the main transport process in all the used transport models. Dispersion is explicitly modelled using a dispersion length or random component in the particle tracking by the CRIEPI, JNC/Golder, Nagra/PSI, BMWi/BGR, DOE/Sandia and ANDRA/CEA modelling teams. The JNC/Golder and Nagra/PSI teams also included several discrete pathways which gives rise to dispersion. The Posiva/VTT team used an implicit description of dispersion obtained from particle tracking in a heterogeneous flow field, but added a random component to the particle displacement to enhance



dispersion. It was judged that the description of the flow field was not detailed enough to simulate local scale velocity variations. The two SKB teams have only considered the hydrodynamic dispersion implicitly due to the presence of several flow paths with different residence time.

Considerable model development has taken place to better describe the effects of matrix diffusion and sorption. Five of eight modelling teams considered matrix diffusion and sorption in the predictions of the STT-1 tracer test. The remaining teams modelled only surface sorption. During the evolution of the tasks it was found that matrix diffusion needed to be incorporated in order to simulate the tails of the breakthrough curves. Thus, for the prediction of STT-2 all of the modelling groups had incorporated matrix diffusion and sorption. Although the principle for matrix diffusion is similar in all models it is implemented in very different ways, where most models are based on solving the diffusion equation. The ANDRA/CEA, BMWi/BGR, CRIEPI and Nagra/PSI teams consider matrix diffusion in a limited matrix penetration depth. The Nagra/PSI team furthermore can take into account matrices with different properties. The implementation of the JNC/Golder, Posiva/VTT, SKB/KTH-TRUE and SKB/KTH-ChE teams assumes an infinite matrix. The approach applied by the DOE/Sandia team is based on the use of distribution of mass-transfer rates where a limited penetration depth is implied, although it is not explicitly given as a parameter. The method for choosing parameters for matrix diffusion and sorption is discussed in Section 5.3.

Most modelling teams have included surface sorption in addition to matrix diffusion and matrix sorption. The exception is the SKB/KTH-ChE team that in their predictions only consider matrix diffusion and sorption. However, in their evaluation work the effect of surface sorption was studied. All team have considered surface sorption as a linear equilibrium process except the SKB/KTH-TRUE team which has included a kinetic effect for representing the sorption on the fracture gouge material.

All transport models include assumptions of the relationship between the surface area available for surface sorption and matrix diffusion, and the water flowing in the fracture. The relationship is not always explicitly stated, but inherent in the assumption used concerning flowpath geometry. Several teams have studied this relationship in detail. Their models rely on that constant effective relationship between surface area available for sorption and matrix diffusion and the water flow may be derived for a flow path. This can for example be expressed as the LW/Q-parameter group used by the SKB/KTH-ChE team, the  $\beta$ -parameter used by the SKB/KTH-TRUE team and the  $u$ -parameter used by the Posiva/VTT team. In Section 5.3 an overview of the used values is given.

Several of the modelling groups also considered diffusion of water into zones with immobile water (SKB/KTH-TRUE, Posiva/VTT, JNC/Golder). Tracers are in this case able to diffuse from the flowpath into adjacent areas of the fracture with stagnant water. Thus, the area available for diffusion depends strongly on the flowpath dimensions a factor that is largely unknown.

### *Numerical approach*

Modelling of advection-dispersion with matrix diffusion in a two-dimensional geometry requires large computational efforts if it is performed explicitly. A geometrical description is required of the fracture as well as the matrix blocks, thus resulting in a three-dimensional geometry. Large differences in time constants for fracture elements and matrix elements often lead to numerical problems and extreme computation times. The three-dimensional approach was used by the CRIEPI team and the BMWi/BGR team in their simulations of STT-1. In the predictions of the two last tracer tests, the BMWi/BGR team simplified their model by treating the matrix as an independent 1D structure, thus significantly reducing the number of connections in their model.

The other modelling teams have reduced the transport modelling to a 1D-problem by applying a streamtube or pathline approach. This approach assumes that transport occurs through independent flowpaths with negligible interaction between the flow paths. Various methods have been used to derive the length, width and water flow within these streamtubes, simple hydrological modelling, particle tracking and pathway analysis. The transport within each flowpath either by explicitly modelling the fracture and the matrix block, e.g. ANDRA/CEA, or using a dual-porosity approach.

Several teams (e.g. the SKB teams, Posiva/VTT) have made use of the linear nature of the transport equation to simplify the problem. Analytical functions have been derived that describes the effects of matrix diffusion and sorption, Taylor dispersion in the fracture and kinetic surface sorption. By using convolution techniques the combined effect of several processes may be simulated for a case with a complex source term.

## **5.3 Model parameters**

### *Hydrology*

The hydrological parameters used for modelling of Feature A are based on the results of performed site characterisation and the evaluation of previously performed tracer tests. Thus, the modellers have a large database and considerable experience in deriving hydrological parameter suitable for their models. The modelling groups have thus only made minor modifications to the data used in Task 4C and 4D.

### *Transmissivity - Conductivity*

The ANDRA/CEA models used a constant transmissivity for Feature A corresponding to the geometric mean of the measured transmissivities in the boreholes  $\log T = -7.44$ . Nagra/PSI used a fracture conductivity of  $7.1 \cdot 10^{-4}$  m/s derived from the DP1-DP4 tracer tests.

In the homogeneous cases JNC/Golder used a transmissivity in Feature A of  $7 \cdot 10^{-8}$  and  $1.25 \cdot 10^{-7}$  m<sup>2</sup>/s in the STT-1 and STT-2 test, respectively, based on an analysis of the flow logging in the boreholes from Dershowitz et al. (1996) and an evaluation of

Task 4D. In the heterogeneous cases the transmissivity field was conditioned on the values in the boreholes measured in the pressure build-up tests.

CRIEPI have evaluated the transmissivities in the borehole section by calibrating against observed drawdown in the preceding tracer tests. The transmissivity field is assumed to have a lognormal distribution. This approach results in a considerably higher transmissivity in KXTT3 than obtained from other measurements.

The BMWi/BGR team calibrated the hydraulic conductivity in the areas around the boreholes to fit the measured drawdown in the previously performed tracer tests using an iterative trial and error technique. The fracture aperture was kept constant throughout the feature. The calibration resulted in an increased transmissivity around boreholes KXTT2, KXTT3 and KXTT4, a slight decrease around KXTT1 and a considerably lower value around KA3005A.

The Posiva/VTT team started using a transmissivity distribution with a  $\log_{10}$  mean,  $m_Y$ , of -8 and a standard deviation of 1. Calibration on the measured drawdown in ten previously performed tracer tests indicated that the mean transmissivity should be higher. A mean of the  $\log_{10}$  transmissivity of -6.8 was used for the predictions. Based on the head differences and mean transport time in the preliminary tracer experiment it was concluded that a suitable value for the standard deviation would be between 1.5 and 2.0. However, due to numerical difficulties the simulations were performed using a standard deviation of 1. No conditioning of the transmissivity field to the measured borehole transmissivities was made.

The SKB/KTH-TRUE team used the geometric mean of the transmissivity of the borehole sections ( $m_Y = -7.7$ ) estimated from the pressure response in the interference test. These estimates were different from those given in Winberg (1996) due to a different evaluation model. A variance derived from the transmissivity of the borehole sections ( $\sigma^2_Y = 0.4$ ) was used. However, the conditioning procedure changed the transmissivity statistics giving a higher mean and variance.

In the channel network model used by the SKB/KTH-ChE team, the conductances of channels belonging to Feature A were assigned a distribution with a mean value which matches a transmissivity of  $1.4 \cdot 10^{-7} \text{ m}^2/\text{s}$ .

### *Correlation length*

Very little information on the correlation length was available for the modellers. As a first approximation a correlation length of 0.3 - 0.4 m was assumed in the site characterisation report (Winberg, 1996). This value was based on the dispersivity obtained in the preliminary tracer test. The Posiva/VTT team used a value of 0.4 m, while the SKB/KTH-TRUE and the CRIEPI team used a correlation length of 1 m.

### *Fracture aperture*

The fracture aperture is generally based on calibration on the non-sorbing tracer breakthrough in previous tracer tests. BMWi/BGR introduced a fracture porosity. The JNC/Golder DFN-model used transport apertures based on the transmissivity using an

empirical relationship (Uchida et al., 1994) in their predictions for STT-1, but changed it to a constant aperture for the predictions of STT-1b and STT-2. In the stochastic continuum models used by the SKB/KTH-TRUE and the Posiva/VTT team a variable hydraulic aperture was derived from the local transmissivity using the cubic law. However, to correctly simulate the breakthrough curves from previous tracer tests a local transport aperture 9 - 15 times higher than the hydraulic aperture was used. The SKB/KTH-ChE team derived their fracture aperture from the channel conductivity based on the cubic law. The proportionality constant was obtained by calibration on previous tracer tests.

### *Boundary conditions*

Generally, less attention was given to the hydrological boundary conditions than in Tasks 4C and 4D. Tests indicated that boundary conditions had small effect on the tracer flow. Also the background changes in the hydraulic head was smaller between the STT-tests than between the RC-1 and DP1- DP4 tests.

All of the models assumed that the hydraulic head at some distance, roughly 10 to 15 m, from the experimental site was unaffected by the pumping. In most cases the heads were fixed on the boundaries, generally as hydrostatic heads or by extrapolating heads measured in the boreholes before the experiments out to the boundaries.

### *Transport*

Transport parameters were to a large extent given or suggested to the modellers, e.g. the modelling input data set containing sorption coefficients, pore matrix diffusivities, matrix porosity and density derived from laboratory experiments (Andersson et al., 1997; Byegård et al., 1998). Other parameters were evaluated from previously performed tracer tests, flow velocities, dispersion coefficients.

### *Water residence time - Flow velocity*

The water residence time or water flow velocity governs the advective transport of non-sorbing tracers. These parameter were in most cases calculated from the hydrological modelling, and calibrated to values observed in previous tracer tests by fitting the fracture aperture, see above. In the cases where no hydrological modelling has been performed the flow velocity is fitted to values derived from the evaluation of previous tests.

### *Dispersion*

The transport models based on the advection-dispersion model (CRIEPI, BMWi/BGR, JNC/Golder, Nagra/PSI, ANDRA/CEA) have used a longitudinal dispersivity obtained from the calibration on the PDT tracer tests experiments performed in the same flowpath. For STT-1 the values varied between 0.11 to 1.6 m, for STT-1b between 0.12 and 0.9 m and for STT-2 between 0.1 and 1.42 m. In general, the models taking into account an enhanced matrix diffusion (ANDRA/CEA: STT-2 and Nagra/PSI) used values for the dispersivity in the lower range.

### *Flow path dimensions.*

The length and width of the flowpaths are either given as explicit parameters or given implicitly in the geometrical description. In some cases the actual dimensions of the flowpath depends on the solution, e.g. for the models using a 2D advection-dispersion model. The length of the flowpath is always set to a value close to the geometrical distance between injection and pumping boreholes. The width of the flowpath was generally considered to be small (0.05 – 0.1 m), but in some cases surface enlarging effects were considered, e.g. multiple parallel fractures.

Several of the modelling teams include the relationship between the surface area available for surface sorption and matrix diffusion, and the water flowing in the fracture. Since, the flowrate varies this relationship usually also varies and is therefore difficult to compare between models. Instead a comparison is made of the flow wetted surface per volume of water or specific interface area. The SKB/KTH-TRUE team has tested a range of different methods to determine this parameter (in the used terminology  $k_0$ ), arriving at values between 950 and 33 000  $\text{m}^{-1}$ . For the predictions a value of 3400  $\text{m}^{-1}$  was used, derived from correlations of data from simulated streamlines. The SKB/KTH-ChE team uses a flow wetted surface per volume of rock of  $1 \text{ m}^2/\text{m}^3$ , which with the flow porosity used corresponds to a  $k_0$  in the order of 2500 – 3000  $\text{m}^{-1}$ . The Nagra/PSI team gives a specific interaction area corresponding to a  $k_0$  of 7000 to 22 000  $\text{m}^{-1}$ , with the lower value used for the STT-1b predictions. CRIEPI have used fracture apertures corresponding to a  $k_0$  in the range 4000 – 6000  $\text{m}^{-1}$ . JNC/Golder have used fracture apertures corresponding to a  $k_0$  in the range 500 – 10 000  $\text{m}^{-1}$ . In the Posiva/VTT predictions for STT-1 and STT-1b the fracture aperture was depending on the local transmissivity. Based on the transmissivity field the values for  $k_0$  is estimated to be in the range 1000 – 4000  $\text{m}^{-1}$ . In the predictions for STT-2 a fracture aperture of 1 mm was used which corresponds to a  $k_0$  of 2000  $\text{m}^{-1}$ . However, in the transport model a fitted parameter  $u$  containing the value of  $k_0$  was used. BMWi/BGR used an approximately constant fracture aperture of 1.4 mm (locally variable in the range 0.3 - 1 mm) which corresponds to a  $k_0$  of 1400  $\text{m}^{-1}$ .

### *Surface sorption*

The modelling teams were provided with estimates of surface sorption coefficients,  $K_a$ , for Na, Ca, Sr, Ba, Rb, Cs evaluated from batch sorption experiments on crushed material. Most of the modelling teams also used data based on 14 days contact time and the geometric area of the crushed samples for their predictions of the STT-1 test. Exceptions are the SKB/KTH-ChE team that did not include surface sorption in their predictions, the CRIEPI team that used the geometric mean of the values derived after 1 day and 14 days contact time. The BMWi/BGR team modelled the sorption in the fracture as an instantaneous equilibrium sorption on material in the fracture using the  $K_d$ -values from the modelling data set.

In the predictions for the STT-1b and STT-2 tests several modelling groups have modified the surface sorption coefficients by calibration on the previous tests.

### *Matrix diffusivity*

The modelling data set also contained recommended values for the effective diffusivity in Äspö-diorite for the different tracers. These values have been used as a basis for the STT-1 predictions made by the modelling groups including matrix diffusion. The Nagra/PSI group considered diffusion into fault gouge material and for this purpose used an increased diffusivity based on calibration of the Uranine breakthrough in the PDT-3 test and derived values for the other tracer by assuming proportionality to the diffusivity in free water and using a nuclide independent geometry factor.

The effective diffusivity has to a large extent been calibrated in the predictions of the STT-1b and STT-2 tracer tests.

### *Matrix sorption*

The modelling groups were provided with values of matrix sorption coefficients ( $K_d$ ) for Na, Ca, Sr, Ba, Rb, Cs from batch experiments on crushed Äspö diorite, mylonite and altered diorite and from through-diffusion experiments on Äspö diorite. The modelling groups considering matrix diffusion and sorption in their predictions of STT-1 used the  $K_d$ -values derived from the through diffusion experiments. For the predictions of STT-1b and STT-2 many groups derived  $K_d$ -values from calibration on the earlier tests.

## 5.4 Model calibration and development

During the evolution of Task 4E and 4F considerable efforts have been made to improve the predictive capabilities of the used models. The main concern has been the transport of the sorbing tracers. Modifications have been made both of model parameters and in the model itself. A summary of the modifications made is given in Table 5-1.

**Table 5-1 Summary of modifications made to take into account sorbing tracers.**

	ANDRA CEA	BMW BGR	CRIEPI	DOE Sandia	JNC Golder	NAGRA PSI	POSIVA VTT	SKB/KTH- ChE	SKB/KTH- TRUE
STT-1	Surface sorption Matrix diffusion	Sorption on fracture material	Surface sorption		Surface sorption	Surface sorption Diffusion & sorption fault gouge	Surface sorption Matrix diffusion	Matrix diffusion	Surface sorption (matrix diffusion)
STT-1b		+ Matrix diffusion	Increased $K_a$		+ Matrix sorption 2 pathways	+Diffusion in cataclasite 2 pathways Adjusted $D_p$ , $K_a$ , $K_d$	Diffusion into stagnant zones	Increased $K_d * D_e$	+ Diffusion into fault gouge & stagnant water
STT-2	Increased $D_e$ & specific surface	Increased $K_a$ , $K_d$	+ Matrix diffusion Adjusted $K_a$ , $K_d$	Total capacity for mass transfer from STT-1	Adjusted $K_d$ Stagnant zones 9 pathways	Adjusted diffusivities and $K_d$	Adjusted $K_d$ , $K_a$ Channels with varying velocity	Reduced flow rate in flow path	Enhanced diffusion sorption factor

Most of the modelling groups had participated in Tasks 4C and 4D and had thereby considerable experience in predicting non-sorbing tracer transport in Feature A. Before the predictions of STT-1 the modelling groups had also the results of the preliminary

design tests with non-sorbing tracers (PDT-1, PDT-2 and PDT-3). Laboratory measurements of sorption coefficients and matrix diffusivities for relevant materials were also distributed. However, no tracer test data were available for calibration of the sorbing tracers. After the predictions of STT-1 were submitted, the experimental results were revealed. Generally, the predictions for the non-sorbing tracers were close to the experimental results. However, many modelling groups had problems representing the tailing observed in the experiment. For the sorbing tracers the predictions generally underestimated the breakthrough time. In the evaluation work the modelling groups revised their models to obtain a better fit. Matrix diffusion and sorption were included in models that previously had only considered surface sorption or linear equilibrium sorption on fracture material. In some cases parameters were modified to enhance the effect of matrix diffusion and sorption. The JNC/Golder modelling group introduced multiple pathways to account for the observed tailing. Nagra/PSI included a second fracture type in order to account for the fast tracer breakthrough observed, especially for the moderately sorbing tracers barium and rubidium.

In the next step, the results of the model development were applied to the prediction of the STT-1b test. Considerable improvement was achieved, but still most of the modelling groups underestimated the breakthrough time for the more sorbing tracers. In the subsequent evaluation, further model calibration and development was performed. It was apparent that the laboratory values for sorption and matrix diffusion could not predict the sorbing tracer breakthrough without adjustment. Alternatively, the surface area available for surface sorption and matrix diffusion was much greater than originally expected. Also alternative processes were investigated, such as diffusion into zones with stagnant water.

Task 4F involved predictions of the STT-2 tracer test. This test was performed in the same flowpath as STT-1 from which the modelling teams had results for sorbing tracers. All of the modelling groups had now included matrix diffusion and sorption. Furthermore, sorption coefficients and/or diffusivities were calibrated on the results of the previous tests. As a consequence, the predictions of the sorbing tracer were in general agreement with the experimental results, see Figure 4-3. A summary of the modelling groups' usage of the data delivered for STT-2 is given in Table 5-2.

A good example of how geological information was used in the modelling is the work performed by the Nagra/PSI team. When setting up the model for prediction of the STT-1, the team found that the large amount of tailing observed in preliminary design test PDT-3 could not be explained by the low values of matrix diffusivity and porosity obtained from the laboratory measurements on Äspö-Diorite. A matrix form with considerably higher diffusivity and porosity must be present. Based on experiences from the Grimsel site in Switzerland and structural geological investigations performed at Äspö (Mazurek et al., 1996), they concluded that presence of fault gouge could explain the breakthrough seen in the tracer tests, i.e. crushed and ground-up rock produced by friction between the two sides of a fault. However, no data were available for sorption and diffusion in the gouge material, and sorption was thus extrapolated from the measurements on Äspö-diorite and the diffusivity evaluated from the breakthrough of non-sorbing tracers in previous tests. The initial predictions were good for non-sorbing and weakly sorbing tracers, but tended to overestimate the breakthrough time for the

more sorbing tracers such as Rb and Cs. As a consequence of this the interpretation of the geological model was revised and flowpaths also interfacing cataclasite were included for the predictions of STT-1b and STT-2. The approach used by Nagra/PSI was also to some extent adopted by other modelling teams, e.g. the SKB/KTH-TRUE and the Andra/CEA teams.

**Table 5-2 Summary of the modelling team's usage of the delivered data.**

Modelling group	BMWi/ BGR	CRIEPI	NAGRA/ PSI	POSIVA/ VTT	SKB/ KTH-ChE	SKB/ KTH- TRUE
Task	SST-2	STT-2	STT-2	STT-2	STT-2	STT-2
<b>Data delivery No 1 for task No 4F Dec 98:</b>						
Updated structural model of the TRUE-1 block and detailed description of Feature A. Technical Memo, TASKS 4E/4F	X		m	X	p, M	P
Structural geology of the TRUE-1 site	X	-	P	-	M	X
Fracture orientation	X	-	-	-	M	X
Fracture intensity	X	-	-	-	M	X
Parameters for DFN modelling	-	-	-	-	X	X
Structural model of the TRUE-1 Block	-	-	m	X	M	X
Hydraulic head	P	P	p	m	p	P
Cross-hole interference data	M	-	X	-	P	X
Groundwater flow data from tracer dilution tests	P	-	X	-	P	m
Results of transport experiments	P	P	P	P	P	P
Conceptual model of Feature A	X	M	m	m	M	P
Transport parameters from the laboratory Diffusivity	P	P	X	P	P	P
Transport parameters from the laboratory Distribution coefficients	P	p	X	P	P	P
Transport parameters from the laboratory Porosity	p	P	X	P	P	P

Notes:

**P** = data of great importance for quantitative estimation of model parameters

p = data of less importance for quantitative estimation of model parameters

**M** = data of great importance used qualitatively for setting up model

m = data of less importance used qualitatively for setting up model

X = data useful as general background information

- = data not used

In their evaluation of the Task 4E and 4F experiments the SKB/KTH-ChE team found that the retardation caused by diffusion into the rock matrix and sorption within the matrix needed to be about 30 times larger than was obtained in the predictions based on the laboratory data (Moreno, 2001). Several possible explanations for this were investigated. With the relationship used to model the matrix retardation effect this implies that the product of the matrix sorption coefficient and the matrix diffusivity needs to be 900 times larger, or that the interaction area between the matrix and the flowing water needs to be 30 times larger. An evaluation of the sorption experiments was made considering also new data available on the sorption on mylonite, altered Äspö diorite and altered fine grained granite (Byegård et al., 1998). The equilibrium sorption coefficients were estimated based on the fraction sorbed and the contact time of the batch sorption experiment. This resulted in matrix sorption coefficients that were 10-25 times higher



for most tracers and 500 times higher for Cs. Thus, this could not be the only explanation for the difference between predictions and observations. It was further noted that the altered rim zone of the fractures was found to have an increased porosity. Values between 2 - 3% were estimated for the part of the zone accessible to the tracers during the tests. This would imply a matrix diffusivity 10-20 times larger than measured in the rock mass. An alternative explanation would be if the flow rate in the transport path was less than predicted or if the ratio flow wetted surface over water flow rate was considerably larger. This could be the case if there is an uneven flow distribution around the extraction section, with a high transmissivity zone conducting most of the water pumped in the extraction section. There are indications of a high conductive zone between KXTT2 and KXTT3. Water from the injection sections may thus travel long distances in Feature A in low flow rate paths before entering the extraction hole or the high conductive zone. Simulations carried out in two-dimensional fractures indicate that a flow rate a factor 5-10 lower is possible.

The SKB/KTH-TRUE modelling team has performed an extensive evaluation of the STT tracer tests (Cvetcovic et al., 2000). In order to simulate the tracer test with the laboratory data on sorption, diffusivity and porosity an enhancement factor for the rock interaction effects needed to be introduced. The value for the enhancement factor is in the range 50 - 65 for the different tracers and tests, i.e. somewhat higher than the enhancement factor of 30 introduced by the SKB/KTH-ChE team. An analysis was made of various explanations for the enhancement factor, which indicated that the rim zone of Feature A may have a 5-10 times larger porosity than the unaltered rock. This may give a factor of a 100 higher effective diffusivity in the rim zone. Also the sorption coefficients in the rim zone were estimated to be 4-50 times larger. The increased retention parameter thus obtained in the rim zone could explain the enhancement factor. The evaluation further indicated that gouge material present in the fracture contributes to the increased retention, but is not of primary importance. The analysis made of flow-wetted surface per volume of water indicated that a very large flow-wetted surface was unlikely and that the value chosen for the simulations ( $3400 \text{ m}^{-1}$ ) is within a realistic range of ( $3000 - 6000 \text{ m}^{-1}$ ). An analysis of the effect of diffusion into stagnant zones concluded that this could cause an enhanced retention, but would not give consistent results for the different tracers.

## **5.5 Lessons learned - Unresolved issues**

### *Experimental site characterisation*

Generally, the experimental site was considered to be well characterised. The need for a detailed characterisation after the end of the test period was emphasised, e.g. the measurement of the spatial aperture distribution of the fracture by a resin experiment. Flow rate measurements were proposed to estimate the sensitivity of the test arrangement to disturbances in the injection or background flow field.

The modelling teams were provided with laboratory measurements of diffusivity and sorption on different rock materials from the Äspö site, such as fresh granite and weakly altered materials. However, several of the modelling teams found that altered material near the fracture surface or fault gouge material had an important role in the tracer retention. The lack of measurements on these materials restricted the possibilities of evaluation of the tracer experiments. Additional measurements of sorption properties of the tested fracture and fracture filling material were therefore strongly suggested.

### *Experimental design*

The experiments were considered well conducted providing a sufficient recovery for analysing the breakthrough. A problem identified by several of the modelling teams concerned the injection technique. The long injection tail obtained due to insufficient exchange influences the tail of the breakthrough curve and thereby hides important information on tracer-rock interaction. Furthermore, the extension of the tail of the breakthrough curve was not monitored long enough to evaluate any limitations of the porous zone available for diffusing tracers.

It was identified that the relatively high pumping rate needed to achieve a reasonable recovery implies short travel times for the tracers. Thus, the interaction with the rock matrix is relatively small. Since most of the used tracers are weakly sorbing, transport is controlled by flow velocity. Suggestions were therefore given to use slightly more sorbing tracers which would be more affected by the interaction with the rock.

Additional suggestions given concerned the use of dipole tests in both the forward and reverse directions.

### *Performance measures*

The performance measures were generally considered sufficient. The final presentation format, which considers tracer flow normalised to total injected mass, makes a consistent intercomparison between different nuclides and between different models possible. It was recommended that a comparison should be made using breakthrough curves calculated for the Dirac source term as well as using the deconvoluted experimental unit response curve for analysis of the tracer test. A suggestion was made to deliver values for the total injected tracer masses as well as for the injection flow rate to avoid unnecessary discrepancies between models and experiments.

### *Suggestions for additional data and analysis*

The suggestions put forward concerned further investigations on the detailed structure of the feature. Information on structural geology on the detailed scale (mm to cm) helps refining a given model and provides limits for transport parameters. Further measurements of the sorptive properties of the rock in the fracture walls and filling material were requested. The difficulty in characterising the fracture with respect to the

details of the flow field was recognised. However, some information could be obtained from measurements of the spatial aperture distribution in Feature A.

*Additional generic research required.*

The modelling teams have also identified areas where additional research is required. These are to large extent related to how to obtain information about the flow-wetted surface and how this parameter can be correlated to the water-flow rate and water residence time. This will require both experimental and theoretical research.

## 6 Conclusions

### 6.1 Tasks 4E and 4F as a testing exercise

The modelling Tasks 4E and 4F were defined with the objectives to develop the understanding of radionuclide migration and retention in fractured rock, and to evaluate the usefulness and feasibility of different approaches to model radionuclide migration of sorbing species based on in situ and laboratory experiments from the TRUE-1 site.

Three tracer tests with sorbing tracers were included in the tasks, all in a radially converging geometry over a distance about 5 meters. Two of the tests (STT-1 and STT-2) were performed over the same flowpath, but with a different pumping rate. The third test (STT-1b) used the same pumping hole, but a different injection hole. The sorbing tracer tests had been preceded by tracer tests using non-sorbing tracers. For each of the two flow paths results from six tracer tests with non-sorbing tracers were available. Thus, a large amount of data on hydrology and non-sorbing tracer breakthrough was available. Laboratory measurements of sorption coefficients and matrix diffusivities for materials from the site were also distributed. However, no tracer test data were available for calibration of the sorbing tracers. In that sense the predictions made of sorbing tracer breakthrough can be considered as "blind".

An important part in the Task 4E and 4F work was the evaluation done after the results of the experiment were revealed. The modelling groups have put a lot of effort in the evaluation, calibrating model parameters, modifying and adapting models and testing alternative approaches. This has proved to be a successful strategy for evaluating the importance of different transport and retardation processes. The interaction with the TRUE project has also proved to be very valuable, where discussions between modellers and experimentalists have provided additional information about geological and geochemical conditions at the site.

The injection method used in the experiment has also been improved. This has resulted in a better-defined source term in comparison with the source term in RC-1 and DP1-DP4 tests modelled within Task 4C and 4D. However, the injection tail that still is present tends to hide information on tracer-rock interaction processes.

The predictions of the sorbing tracer breakthrough in the initial tracer test (STT-1) were not satisfactory. It was apparent that the active processes were more complex than initially anticipated and that the application of laboratory data was not straightforward. As a result of model calibration and modification the predictions were considerably improved for the latter tracer tests (STT-1b and STT-2). During the course of the task, the models also became more similar, concerning the processes that were considered. For the predictions of STT-2 matrix sorption and diffusion was included in all the models, whereas only half of the modelling groups used matrix diffusion and sorption in

their predictions for STT-1. However, there were still substantial differences between the different models used for the prediction of STT-2.

Task 4E and 4F has proved to be very valuable in increasing the understanding of non-sorbing tracer transport in fractured rock. There is a general consensus on the major processes responsible for transport and retardation and also how these processes can be described in a mathematical model. However, there are still a number unresolved questions concerning the application of laboratory data to tracer tests, the extrapolation of tracer tests to other distances and time scales and the application of results to other sites.

## 6.2 Modelling and data

Several different types of models were used within Task 4E and 4F. The models were generally process oriented where the effect of transport and retention processes could be derived from the provided laboratory measurements. The DOE/Sandia model used a somewhat different approach using a statistically distributed diffusion rate coefficient determined by parameter estimation. The diffusion rate coefficient is a lumped parameter, but can be examined in order to compare with laboratory data.

The coupling between the hydrology modelling and the transport modelling is done several different ways, depending on the model structure. The CRIEPI and BMWi/BGR teams solve both hydrology and transport in the same computational grid. The advantage of such a method is the direct coupling between hydrology and transport, which could be valuable in two-dimensional flow-fields. However, the method is computationally demanding and also makes the incorporation of new transport processes difficult. As an example the inclusion of matrix diffusion requires grid modifications, the use of two types of matrix materials would result in very complex geometry. The SKB/KTH-ChE team solves hydrology and transport in the same discrete representation of channels. Transport within each segment is then treated as a one-dimensional problem. The particle following technique used to account for tracer retention is very efficient, but the tracer retention model is not readily adjustable, e.g. by introducing limited diffusion depth. The method deriving discrete flowpaths from streamtubes or streamlines used by the SKB/KTH-TRUE, Posiva/VTT, JNC/Golder, Nagra/PSI teams is efficient and allows for a transport model including a number of retention processes. This approach relies on a number of assumptions, e.g. that the mixing between the pathlines is small.

The work with in Task 4E and 4F has identified a number of problems related to the transfer of laboratory data to field scale experiments. Laboratory measurements have been made on samples from the studied feature. However, the heterogeneity of Feature A adds uncertainty to the evaluation. This concerns the various rock types with different mineralogy and porosity that are in contact with the flowing water along the fracture, and also the variation that is expected in the rim zone of the fracture. Within the time scale of the performed tracer tests only a fraction of a millimetre of the rock will be available for interaction for the more strongly sorbing tracers and only a few

millimetres for the weakly sorbing tracers. There is indications that there is a strong gradient in porosity in the rim zone and thereby also in diffusivity and sorption properties. This has been acknowledged in the TRUE-1 programme and methods to characterise the rim zone has been developed. However, there are still unresolved issues in how to define effective parameters for diffusion and sorption in an adequate way.

### **6.3 Perspective to future tasks**

The modelling Tasks 4E and 4F dealt with transport of sorbing radionuclides in a single feature over distances of 5 metres. The time scale of the tracer tests extended to at the most a few months. The transfer of the information obtained from this work to a performance assessment scale requires extrapolation in time and space. Furthermore, many of the important radionuclides considered in performance assessment are considerably more sorbing than the most sorbing tracers used in the TRUE-1 tests.

The relatively strong retention observed in the TRUE-1 sorbing tracer experiments are believed to a large extent depend on alterations in the rim zone of the fracture leading to an increased matrix porosity, diffusivity and sorption. Thus, the sorbing tracer retention could not accurately be predicted by direct application of the provided laboratory data. Since the importance of the rim zone will diminish with time it may still be appropriate to apply laboratory data to performance scale modelling. However, the modelling performed in Tasks 4E and 4F were not conclusive concerning to what extent the increased retention could be attributed to enhanced matrix mass-transfer. Alternative explanations have been put forward, e.g. that the increased retention to some extent is caused by a large ratio between the surface area available for matrix diffusion and the flow rate, or that velocity field in the channels is very heterogeneous leading to the formation of stagnant zones. These alternative explanations will give very different results when extrapolated to performance assessment scales.

Investigations in how to use site characterisation investigations for performance assessment is important for the future licensing of deep underground repositories. Further investigations of sorbing tracer transport on larger scales will provide additional information on how to extrapolate data. In the TRUE Block Scale experiment tracer tests have been performed in connected fractures on a scale up to 50 metres. In the planned Task 6 flow and transport at two spatial scales will be modelled for both site characterisation conditions and for conditions relevant to performance assessment. The overall objective of Task 6 is to provide a bridge between site characterisation and performance assessment approaches to solute transport in fractured rock. The work performed within Task 4E and 4F constitutes an important basis for this task.

## **7 Acknowledgements**

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## Appendix 1 Data distributed to modelling groups

### Task 4E: Data distribution 1 to 6:

#### Data delivery no 1:

- Data set for PDT-1 and PDT-2 (breakthrough and injection curves for Uranine and Amino G) and hydraulic data (head and pump rate ) as well as electrical conductivity of pumped water.

#### Data delivery no 2:

- Data set for PDT-3 (injection and breakthrough curves for Uranine) and injection data for STT-1.

#### Data delivery no 3:

- Data set for PDT-4 (breakthrough curve and injection curves for Uranine) and for STT-1 (breakthrough curves).

#### Data delivery no 4:

- Report “Preliminary design tests for test with radioactive sorbing tracers (PDT-1, PDT-2, PDT-3)” Progress Report HRL 98-13 (Andersson et al., 1998a)
- Report “Tracer tests with sorbing tracers, STT-1” Draft (Andersson et al., 1998b)
- Data file: Injection concentration versus time for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{58}\text{Co}$ , STT-1b
- Pump flow rate

#### Data delivery no5:

- Report “Radially converging tracer test, RC-3” PM, (Andersson, 1998c)
- Data file: Injection concentration for Uranine, RC-3
- Data file: Breakthrough concentration for Uranine, RC-3
- Pump flow rate

#### Data delivery no 6:

- Data file: Breakthrough concentration for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{42}\text{K}$ ,  $^{85}\text{Sr}$ ,  $^{86}\text{Rb}$ ,  $^{58}\text{Co}$ , STT-1b

- Data file: Hydraulic head, STT-1b
- Pump flow rate

**Task 4F: Data distribution 1 to 2:**

Data delivery no1:

- Report “Updated structural model of the TRUE-1 block and detailed description of feature A” Draft version
- Data file: Injection concentration for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{131}\text{Ba}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$  and  $^{137}\text{Cs}$ , STT-2

Data delivery no2:

- Data file: Breakthrough concentration for Uranine, HTO,  $^{82}\text{Br}$ ,  $^{22}\text{Na}$ ,  $^{47}\text{Ca}$ ,  $^{85}\text{Sr}$ ,  $^{131}\text{Ba}$ ,  $^{133}\text{Ba}$ ,  $^{86}\text{Rb}$  and  $^{137}\text{Cs}$ , STT-2
- Data file: Hydraulic head, STT-2
- Pumping flow rate

## **Appendix 2 Questionnaire**

## APPENDIX 2 COMPILATION OF ANSWERS TO QUESTIONNAIRE CONCERNING TASK 4E AND 4F

QUESTION	CRIEPI	JNC/Golder	Nagra/PSI	SKB KTH-ChE	POSI/VANT	BMWI/BGR	SKB (KTH-TRUE)
<b>1 Scope and Issues</b> <b>a What is your purpose of participation in Task 4E &amp; 4F?</b>	The purpose for our participation in Task 4F was to deepen our understanding of migration phenomena of sorbing solutes in a fracture and to assess the usefulness of our developed numerical codes, FEGM and FERIM, for the prediction of such phenomena..	The goal is to improve the understanding of sorbing and conservative tracer transport at the 5 to 10 meter scale in single fractures and simple fracture networks.	Improve our understanding of radionuclide transport through fractured crystal-line rock. Obtain information on differences and similarities between Aspö and Grimsel conditions. Find out how to up-scale to field conditions the values for transport parameters obtained in small-scale laboratory experiments. Get information on different modelling approaches applied to the same tasks.	Our main interests in Task-4 E & 4F was to improve our knowledge about transport of sorbing species in fractured rock and to apply CHAN3D to field experiments with sorbing species thereby testing its capabilities and weaknesses. The different retardation mechanisms in solute transport in fractured media are also addressed here.	Learn more about water flow and single fracture as a basis for flow and transport conceptualisation for performance assessment. Carefully conducted tracer tests in a hydraulically well characterised fracture with accurately measured source terms and varied pumping conditions was expected to reveal essential features of flow and transport processes.	Understand transport mechanisms for different solutes in fractured rock, especially for sorbed and radioactive solutes. Test the numerical models developed jointly by BGR and University of Hannover, Germany. Exchange experience gained from in-situ experiments at the GRIMSEL Test Site	Participated as a part of the TRUE team.
<b>b What issues did you wish to address through participation in Task 4E &amp; 4F?</b>	Address the influence of the rock matrix on the migration of sorbing tracers.	Fracture flow and transport pathways and the sorption and diffusion properties along those pathways –particularly gouge materials within fractures.	Investigate the influence of the radionuclide-rock interaction onto tracer transport. Get information on possible limitations of our relatively simple model for flow and transport.	Obtain a better knowledge of the important entities that influence solute transport: flow distribution, flow porosity and flow-wetted surface.	Flow heterogeneity (channeling), especially flow rate distribution over the fracture plane, to assess the interaction rate of transported solutes with fracture walls in various parts of the fracture.	The influence of sorption effect of sorbing tracer in the fractured rock, e.g. whether the physical kd concept is suitable to describe the fast chemical reaction (mass equilibrium reaction).	Understanding of mass transfer processes in Feature A.
<b>2 Conceptual model and data base</b> <b>a To what extent have you used the data sets delivered?</b> <b>Task 4E: Data Distribution 1 - 3 and 4.</b> <b>Task 4F: Data distrib. 1&amp;2.</b>	Geometry of Feature A and of the boreholes. Transmissivity at the borehole section KA3005A R3. Injection and pumping rates. Drawdowns in injection and withdrawal sections. Hydraulic heads prior to start of PDT-3. Tracer concentration at injection section and breakthrough curves at pumping section. Effective diffusivities for the tracers. Porosity of the rock matrix.	All data was used at least to some extent. The DFN model was based on the data distribution fracture geometry and properties. Simulations were made for the hydraulic and transport response from all of the previous experiments in Feature A.	<b>4E</b> Head distributions. Results tracer test PDT3 Laboratory data from HRL-97-07 <b>Task 4E: DD #4:</b> Only the experimental breakthrough curves were used for the analysis. Hence, there was no application of the delivered head values. <b>4F</b> see table 5.2.	Locations of the Features A and B, the tunnel, niche and boreholes. Transmissivity of Features A and B, hydraulic conductivity of the rock mass and hydraulic head in the features. The data from RC3, DP5 and DP6 used to refine the model. PDT1-PDT3 used to calibrate the model for prediction of STT1a. PDT4 used to calibrate the model for prediction of STT1b.	<b>4E</b> Pumping & sampling flow rates, injection curves, results of the PDT-3 test, provided laboratory data on the sorption properties of the nuclides <b>4F</b> Injection curve, geometrical information on the positions of the injection and pumping boreholes to estimate the length of the transport path, sorption parameters, pumping flow rate, pretests to get the groundwater transit time orders of magnitude.	<b>4E</b> Based on the data delivered in Task 4C/4D we used additionally following data: <b>4E.i:</b> Data Distribution #1-3 <b>4E.iii:</b> Data Distribution #4-5 <b>4F</b> The data sets delivered for the updated structural model mostly agree with the parameter values used in our model, e.g. the calculated mean porosity and hydraulic conductivity values are in agreement over a range of two orders of magnitude.	Almost all data have been used.
<b>b Specify more exactly what data in the data sets you actually used?</b>	Transmissivity at the borehole section KA3005A R3 determined from the flow- and pressure build-up test. Injection and pumping rates during RC-1, 2 DP-1-6, PDT-1-3 and STT-2 Drawdowns in injection and withdrawal sections during RC-1, 2 DP-1-6 and PDT-1-3 Hydraulic heads prior to start of PDT-3 Breakthrough curves at the injection section during STT-1, PDT-2 and STT-2 Breakthrough curves at the pumping section during STT-1 and PDT-2 Effective diffusivities for the tracers Porosity of the rock matrix	The data deliveries were used to provide the fracture network geometry and the properties of Feature A and background fractures. Properties used included diffusion and sorption parameters. Data deliveries of 4E and 4F provided experimental boundary conditions and initial conditions, including the experimental setup and time frames. They also provided tracer tests for previous experiments such as PDT1-PDT3 which were used for conditioning.	Head distributions to determine an averaged natural background head gradient and flow velocity. Calibration to uranine-PDT3 to determine, the flow width, the Peclet number, a lumped parameter describing the effect of matrix diffusion, an estimate of the pore diffusion constant, and a correction factor for deriving the proper injection rate deduced from the measured injection tail. Laboratory data HRL-97-07: $K_{tr}$ (extrapolated to crushed mylonite which was assumed to be closest to fault gouge), $K_{tr}$ , $D_w$ (used to extrapolate the value for $D_p$ of uranine derived from the calibration experiment to other nuclides).	From the data deliveries, the injection and breakthrough data. Experimental set-up, the injection/sampling system for PDT1-PDT3, and hydraulic heads in the borehole sections from data delivery No1. Termination times for STT1b from letter of 8 August 1998. Data delivery No5: diffusion and sorption data for Co and K. <b>4F</b> Injection data for PDT3 and STT2 from the data deliveries. Experimental set-up, the injection/sampling system for the PDT3, and hydraulic heads in the borehole sections from data delivery No1. Termination times for STT2 from letter of 6 April 1999.	Generally, only the injection data of the experiment and nuclide specific laboratory data on the diffusion and retardation properties. In addition, the background head field has been based on the head measurements for the PDT-3 test.	<b>4E</b> For the predictions of STT-1 the measurement of hydraulic draw-down, the information from DP5/6, PDT1/2/3. For predictions of STT-1b the data sets from PDT4, PTT, RC and DP - 1 was used and analysed. <b>4F</b> In the modelling of STT-1 the hydraulic drawdown measurements, data from DP5/6 and PDT1/2/3. For the predictions of STT-2 no other data was used.	<b>4E:</b> The following data sets have been used: Data distribution No. 1: p2inj4.txt, pdf2b4.txt (used for calibrating water residence time distribution). Data distribution No. 2: all the data sets. Data distribution No. 3: all the data sets. Data distribution No. 4: all the data sets. <b>4F</b> See Table 5.2



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<b>c</b> What additional data did you use if any and what assumptions were made to fill in data not provided in the Data Distributions but required by your model?	Ratio of longitudinal dispersivity to transverse dispersivity in Feature A. Longitudinal and transverse dispersivities in the rock matrix. Hydraulic conductivity of the rock matrix. Feature A was assumed to be a single open fracture with constant aperture	Assumptions were made concerning fracture size distribution based on data in other areas of Äspö. Sorption and diffusion properties from data distributions were supplemented by information from reference tables and from the SKB fracture characterization project FCC.	Results of small scale structural geological investigations of bore cores taken close to Feature A were adopted. In addition, the assumption was made that within Feature A similar structures are present (cf. SKB-ICR-97-01, chapter 8.5 and pers. com M. Mazurek).	The hydraulic head at the boundaries in the rock mass was estimated by using scarce data. Flow wetted surface was also assumed, it was considered that the whole (or a fraction) Feature A was open to the flow.	<b>4F</b> Additional data: molecular diffusion coefficient in free water, number of the flow channels, widths of the flow channels. Assumptions: width and aperture of the flow channels are constant, velocity distribution in flow channel is linear.	$K_d$ values and half-life time for every species and their isotope.	Parameters for the kinetic sorption in gauge material obtained in evaluation of STT1 and used for prediction of STT-1b (have been obtained by fitting the calculated breakthrough curves with the measured ones). 4F
<b>3 Model geometry and structural model</b> <b>a</b> How did you geometrically represent the TRUE-1 site and its features/zones?	Only Feature A modelled and its surrounding rock matrix.	The TRUE-1 site was represented as a 3D discrete fracture network model combining deterministic, stochastic, and conditioned features depending on the level of detail available and required. For transport modeling, the fracture network were simplified as tubes of rectangular cross-section with diffusion to linearly connected immobile zones representing gouge, breccia, altered rock, and rock matrix.	By a dual porosity concept with underlying planar fracture geometry using several narrow channels for the flowing water in contact with diffusion accessible porosity (fault gouge, representing a high diffusion accessible porosity, and cataclasis representing a low diffusion accessible porosity).	In the model, the tunnel with the niche, all the boreholes, the Feature A and the Feature B planes were included. The feature A was extended to the boundaries and the feature B fractures were treated as confined fracture planes. The size of the modelled rock volume was 30 x 30 x 40 metres..	<b>4E</b> Only the feature A was modelled. It has been modelled as two dimensional heterogeneous plane. The influences of all the other features intersecting feature A were incorporated only by applying the measured background field of the hydraulic head. <b>4F</b> Model includes only the transport channels.	Based on the structural-hydraulic model the fracture system was analysed using the data from borehole cores and hydraulic tests. Potentially water-bearing fractures were combined into a fracture system described by a 2D planar area. This fracture model was analysed in the Task 4C/D and not changed for 4E/4F. For sorbing tracers a coupled fracture-matrix model was used.	Numerical model discussed below only used to obtain $\beta$ - $\tau$ relationship; non-reactive breakthrough obtained through calibration. Feature A is assumed to be a 2D planar fracture with spatially variable aperture
<b>b</b> Which features were considered the most significant for the understanding of flow and transport in the TRUE- 1 site, and why?	We think that whether Feature A is connected with other fractures or not is the most significant because the flow and transport in the TRUE-1 site depends greatly on the independence of Feature A.	The internal structure of Feature A in terms of pathway width, infillings, coatings, and stagnant zones are the most important for radionuclide retention at the time scale of Task 4. In addition, the pathway geometry itself is important, and is determined both by fracture internal structure and by the geometry of intersecting fractures. For flow, the boundary conditions are extremely important.	Geological structures on the scale of mm to cm which determine mainly the characteristics of water flow, retardation and the distribution of migrating nuclides.	Feature A was the most important because most of the flow and transport occur in that Feature. When the pumping flow rate in the collection section is sufficiently large, most of the injected tracer is recovered. On the other hand, if the flow rate in the collection section is low (or a small drawdown is created in the recollection section) a fraction of the injected tracer may flow into the tunnel. In some cases, the amount of tracer that is transported into the recollection section is small.	Flow field, especially for non-sorbing tracers, since matrix diffusion is not a significant process at high flow rates. Dispersion due to different transit times of the streamlines. Molecular diffusion between streamlines reducing differences in the breakthrough times. Molecular diffusion into stagnant areas of the flow field. Filling material in the fracture with high porosity. Sorption delays breakthrough and amplifies matrix diffusion.	The analysis of geological data and hydraulic tests shows that there is a weekly connection between Feature A and B, and they have quite different hydraulic conductivity. The numerical calculation shows that any hydraulic influence of Feature B on Feature A may be neglected for the configuration used in the tracer tests in Feature A.	Feature A.
<b>c</b> Motivate selected numerical discretization in relation to used values of correlation length and/or dispersion length	We used the correlation length of transmissivity of 1 meter and the longitudinal dispersivity of 1.42 meters; therefore we discretised the region near the boreholes by the square elements of which the length of the side is about 0.2 meters.	Externally, transport pipes are discretized to the level of detail necessary to define the pathway geometry – in our case 9 pipes defining two primary pathways and two minor pathways. These pipes are discretized internally by the PAWorks/LTG code to ensure that the Peclet criteria for convergence for given velocity, pipe length, and dispersion are satisfied.	In our model there is no discretisation scheme in relation to correlation length and/or dispersion length.	It is assumed that the conductance of the channels is uncorrelated in space. Channels lengths taken to be 0.7 m. The impact of the channel length on transport is not important, since most of the transport occurs through only a few channels. The choice of the channel length was, in part, based on the computer capacity. The present model has 114 000 nodes and about 350 000 channels.	<b>4E</b> The discretization was made as fine as possible, because it was assumed that the variations in the flow velocities in the length scale reachable by molecular diffusion are important. In practice computer resources limited the discretization. The element length has been clearly smaller than the applied correlation length. <b>4F</b> Analytical model with no discretisation in space.	The same order of selected finite-element discretisation (0.5 ~ 1 m) in relation to used dispersion length (0.6 ~ 0.9 m) was used.	Correlation chosen based on possible discretization (discretization 0.4 m, input integral scale 1 m).

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<p><b>4</b></p> <p><b>a</b> How did you represent the material properties in the hydraulic units used to represent the TRUE-1 site?</p>	<p>properties</p> <p>See Table 2 and 3.</p>	<p>The conductive structures (Feature A, A', NW-2', etc.) were parameterized in terms of transmissivity for flow, and transport aperture and flow width for transport. Immobile zones were parameterized in terms of reactive surface area, porosity, and thickness. Sorption was described by <math>K_d</math> and <math>K_s</math>.</p>	<p>In our model the flow and transport domain is considered to be a two-dimensional porous medium with an underlying homogeneous and isotropic transmissivity field. For such an approximation the flow field is fully determined by the experimental pumping rates; a value for the transmissivity is therefore not required. Fracture conductivity was taken from the literature without modification (SKB-HRL-97-13, p. 7).</p>	<p>The rock mass and Features A and B are represented as a network of channels. Conductances of channels in Features A and B are taken from a distribution with a mean value matching the measured transmissivity. The mean value for the channel conductance distribution in the rock mass is calculated from the rock mass hydraulic conductivity. Standard deviation is taken from hydraulic measurements at the Aspö site.</p>	<p><b>4E</b> Feature A modelled as a lognormal transmissivity field and spherical correlation function. The transport apertures calculated from hydraulic apertures with fixed coefficient fitted on PDT-3. Sorption properties from laboratory tests. <b>4F</b> Hydraulic properties not used needed since only flow rate through channel is used - estimated from the dilution of the injection curve. Groundwater transit time estimated from STT1. Sorption properties and diffusion and porosity of the rock matrix based on laboratory data. Total width of channels based on injection borehole diameter.</p>	<p>The three parameters hydraulic conductivity, fracture aperture and storage coefficient are important for representing hydraulic behaviour in the fracture system. Saturation with water at the TRUE-1 experimental site was assumed, and the hydraulic conductivity and fracture aperture were varied in our models according to the hydraulic drawdown available from tracer tests.</p>	<p>(See Tables)</p>
<p><b>b</b> What is the basis for your assumptions regarding material properties?</p>	<p>Transmissivity in a fracture is generally considered to show a normal distribution in the logarithmic scale and to distribute spatially with correlation.</p>	<p>Fracture transmissivity was derived from the hydraulic tests during the rock characterization stage, including flow logs, packer tests, and hydraulic interference. Transport properties were based on laboratory measurements in the MIDIS database, with some adjustments for calibration to previous tracer tests in the rock block. Immobile zone thickness and porosity were based on information on the fracture micro-structure, combined with calibration to tracer test results</p>	<p>Values for transport parameters obtained in small-scale laboratory experiments had to be re-scaled to field conditions and were used without further changes for the predictions of the STT1 tracer test. After the analysis, the best-fit parameter values were applied to new predictions of the STT2 tracer test. They still had to be consistent with laboratory values, otherwise this was considered to be indicative of failure of the model. Values for the flow width, the Peclet number, the specific interface area fracture/porous matrix had consequently to be the same for all the tracers in a given experiment. Scaling factors ("fudge factors") or further parameters with no physical background to reproduce measurements were consequently excluded.</p>	<p>The assumptions are based on geometrical considerations and observations that fluid flow and solute transport occur through channels in fractured media. Diffusion and sorption constants are taken from laboratory experiments.</p>	<p><b>4E</b> A lognormal transmissivity field is a common approximation based on a large number field and laboratory studies. Separate transport and hydraulic apertures were needed due to numerical difficulties in solving the head field with a large variance of transmissivity. For the sorption properties there was no other source of information than the laboratory data. <b>4F</b> Assumed that the same flow path and channels are activated as in STT1 and that changes in the background field were small. Thus, groundwater transit time was directly scaled using the pumping rates of the tests. The total width of the channels based on the diameter of the borehole. Assumed that passive injection cannot spread the tracers to much larger area than the diameter of the borehole. To some extent the channel widths can be calibrated on STT1.</p>	<p>The storativity has been assumed to be zero if gas saturation in the pores and water compressibility can be neglected when the hydraulic pressure in the experiments did not differ from the natural conditions.</p>	<p>Hydraulic-structural investigations may be interpreted such that "A" is singular well-connected feature and less-connected with the surrounding.</p>

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<b>c Which assumptions were the most significant, and why?</b>	Spatial correlation of T since it is a prerequisite for kriging	For transport, the most significant assumptions are those related to the immobile zones – immobile zone volume, porosity, and reactive surface area. These values determine the strength of surface sorption and matrix sorption, and ultimately the shape of the breakthrough.  The other key assumption is the geometry of the fracture network and internal structure of "Feature A", which determine the geometry of transport pathways.	See comments above.	The most important assumptions are the properties of the Features A, and B, as most of the water flows through these Features. Sorption was very important in the tracer test with Caesium.	<b>4E</b> For tracer breakthrough and drawdowns: the use of a single fixed number fitted to PDT3 as ratio between the hydraulic and transport apertures. This is probably valid only for the flow path and test configuration where it was derived. For the sorbing tracers the assumption that the laboratory values are directly applicable to Feature A governs the results. <b>4F</b> For non-sorbing tracer and for the estimation of the first arrival times and the assumptions concerning maximum groundwater flow velocity are important. For sorbing tracers the total flow rate and the width of the channel is most significant since it determines the strength of the interaction with the surrounding rock.	In the homogeneous model the fracture aperture was often considered as a constant. Actually this is a most significant factor, which influences the distribution of flow field on the one hand, and consequently the transport velocity of tracer on the other hand. As increasing experimental information became available, a heterogeneous model with local varied fracture conductivity and aperture has been built.	Assumption of singular feature most significant, if wrong the approach is questionable and obtained understanding may be misleading.
<b>5</b>	<b>Boundary conditions</b>						
<b>a What boundary conditions were used in the modelling of the TRUE- 1 tests?</b>	See Table 2 and 3.	Boundary conditions for flow are fixed heads on a 50 m scale cube. Transport boundary conditions are given by the experimental rates of injection and pumping, as a group flux to the fractures in the pumping and injection intervals.	A constant head distribution far away from the pumping and recharging well of the dipole.	Given hydraulic heads are used as boundary conditions on the vertical sides, on the top and on the bottom. The hydraulic head in the tunnel is also taken as boundary condition. The extraction flow rates in the pumping well was considered. A skin factor is used which gives a lower conductivity of fractures close to the tunnel.	<b>4E</b> Fixed hydraulic head boundary conditions extrapolated by fitting a linear model into the measured fresh water head values in the natural flow conditions prior to PDT3. <b>4F</b> The measured flow rate from the injection curve and the estimated groundwater transit time.	The piezometric head at all boundaries of Feature A. The Neumann-boundary condition flow rate was used for simulating injection and pumping. The boundary conditions were determined in task 4C/4D and assumed the natural flow conditions were not changed, although the measured hydraulic head shows a transient situation.	<b>4E</b> Linear head change along all four boundaries. <b>4F</b> Constant head $h=-46.5$ for all boundaries
<b>b What was the basis for your assumptions regarding boundary conditions?</b>	The hydraulic heads at the points distant from the pumping or injection section are dominated not by pumping but mainly by the natural hydraulic gradient. The distance between the surrounding boundaries and the pumping or injection section is more than 10 meters. And the thickness of the modelled rock matrix is 0.1 meters. So we do not think that the tracers reach the any boundaries.	Hydraulic boundary conditions were based on the calibration of the DFN model to observed hydraulic interference and head measurements. The transport boundary conditions were specified in the experiments.	The convenience of obtaining analytical solutions in the frame of the streamtube for-malism.	In the rock, the pressure is almost constant, decreasing slightly in the tunnel direction. Most of the pressure difference is found around the tunnel	<b>4E</b> Assumed that Feature A is a large fracture and that the intersections with other hydraulically active fractures are not close to the test area. <b>4F</b> Assumed that the flow rate calculated from the injection curve represents the flow rate through the transport channel. Assumed that the background flow field does not influence too much on the test so that it is possible to scale the flow velocity from earlier tracer test with a different pumping rate.	For our calculations, we used an area for the fracture plane that is twice as large as the experimental site, so we assumed the boundary conditions at the outer boundary have no influence on the simulation. The boundary conditions were extrapolated from the natural hydraulic head distribution measured in the boreholes.	<b>4E</b> The boundary conditions are obtained using the measured head values and drawing some rough isolines of head out to the boundaries. <b>4F</b> The boundary conditions are obtained based on the measured head values.
<b>c Which assumptions were the most significant, and why?</b>	That the hydraulic heads on the surrounding boundaries of the model never change during the tracer tests, because the natural hydraulic gradient influences tracer recovery significantly.	The assumed head boundary conditions significantly influences transport pathways.	No additional assumptions were made.	The most significant assumption was the extent of Feature A. It is assumed that Feature A reached the borders of the model. If it is assumed that the Feature A is limited and does not reach the borders, an unrealistic drawdown is obtained.	<b>4E</b> The extrapolated fixed head boundary conditions not valid if there are intersections with well-conducting fractures close to the pumping hole. <b>4F</b> For interaction with the surrounding rock the assumption that the flow rate per channel width can be estimated using the flow rate from the injection curve and borehole diameter as channel width is most significant.	It was important to use the correct pumping rate in the model because it determines the flow configuration.	Boundary conditions not crucial since conservative breakthrough obtained through fitting. An important assumption is though that the flow field is constant during the whole experiment, i.e., the conservative breakthrough is valid for the longer time scales of the sorbing tracers.

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<b>6 Model calibration</b> <b>a To what extent did you calibrate your model on the provided hydraulic information? (steady state and transient hydraulic head etc.)</b>	We calibrated our model on the following hydraulic information. - Drawdowns in injection and withdrawal sections during RC-1,2 DP-1,6 and PDT-1-3 - Hydraulic heads prior to start of PDT-3	The hydraulic model was not calibrated to hydraulic information in the sense of inverse modelling. However, the model parameters were derived from all the hydraulic test information, including both steady state and hydraulic interference testing.	No calibration was performed on hydraulic data.	Boundary conditions and transmissivity of the features A and B were estimated from the hydraulic information (steady state)	<b>4E</b> The realisations of the transmissivity field were selected by simulating a large set of the earlier tracer tests. Drawdown in PDT3 used to calibrate the ratio between the hydraulic and transport apertures. <b>4F</b> Model calibrated to reproduce measured total flow rate through the transport channel and the first arrival time in the STT1-test	We calibrated our flow model with a constant hydraulic head under the natural flow conditions and under the conditions of almost all tracer tests, which were performed with different injection and pumping rates.	a) Fields conditioned on head prior to pumping and during pumping in RC-1 experiment
<b>b To what extent did you calibrate your model on the provided "transport data"? (breakthrough curves etc.)</b>	We calibrated our model on the breakthrough curves at the pumping section during STT-1a and PDT-2..	The immobile zone transport properties were calibrated based on previous in situ transport experiments. However, in most cases, sorption properties ( $K_d$ and $K_a$ ) were used directly from the MDS database.	Calibration of transport was done by inverse modelling of the former STT1 tracer breakthrough curves	Void volume of the "A" used in RC-1 was determined from the preliminary design tests. PDT3 was used to obtain void volume for the tracer test STT1a and PDT4 for STT1b. The void volume for the tracer test STT2 is obtained from PDT2.	<b>4E</b> The breakthrough time in PDT-3 used to calibrate the ratio between the hydraulic and transport apertures. <b>4F</b> Breakthrough curves of STT1 used to calibrate the first arrival time (maximum flow velocity in the transport channel) and sorption parameters ( $K_a$ ).	The flow model was calibrated using the measured hydraulic heads. The transport model, which is based on the flow model, was calibrated using the breakthrough curves from tracer tests (breakthrough time, maximal concentration and tailing form of the curve).	The moments of $g(r)$ obtained by calibrating the breakthrough curves using the PDT3 and PDT4 for 4E and PDT2 for 4F. The factor $f$ for $\tau$ and $K_{sp}$ and $\alpha$ for the kinetic sorption in the gouge material obtained by calibrating breakthrough curves from STT-1 and STT-2 (4F).
<b>c What parameters did you vary?</b>	Hydraulic head at the surrounding boundaries - Transmissivity, aperture, dispersivity and surface related sorption coefficient in Feature A - Dispersivity and sorption coefficient in the rock matrix.	Immobile zone thickness and porosity, and the ratio of flow width to transport width were varied.	In the analysis of the STT1 tracer test the following parameters were varied: The flow width (cf B); the Peclet number (Pe); the parameter "matrix diffusion time" ( $\tau_0$ ); and the parameter "matrix propagation time" ( $\gamma$ ).	PDT1-PDT3 used to recalibrate the model. The skin factor used to limit the water flow into the tunnel was varied in some simulations to match the recovery of the tracer. A small skin factor means that a larger fraction of the injected tracer is transported into the tunnel. The transmissivity of Feature A was varied to match the drawdown.	<b>4E</b> The variance of the transmissivity field was varied during calibration. In the calibration of the transport properties only the ratio between the transport and hydraulic aperture was varied. <b>4F</b> Number of parallel channels and channel widths. Also $K_a$ was varied in the calibration runs of the STT1-test.	The local distribution of hydraulic conductivity and fracture aperture as well as effective porosity, dispersivity and diffusion were varied for single elements in Task 4C/4D. Since then, only slight changes have been made.	c) The matrix diffusion and sorption parameter ( $k$ ) has been increased approximately 40 times.
<b>d Which parameters were the most significant, and why?</b>	Sorption coefficients are most significant because the tracer travel time greatly depends on the values of the coefficients..	Immobile zone porosity, volume, and reactive surface area determine the strength of matrix and surface sorption, given the use of laboratory values of $K_d$ .	For our flow part of the model the correct application of the pumping rate ratio was essential because it mainly determines the flow field. (The perturbation due to the natural background flow field and, hence, its parameters, could be nearly neglected as a consequence of the high pumping rate downstream). For a conservative tracer cf B mainly defines the peak arrival time. The Peclet number affects the peak width. $\tau_0$ affects the trailing edge, and $\gamma$ affects the time of the breakthrough tail-end perturbation. Every parameter has its own impact on the tracer breakthrough and has an effect on different parts of a breakthrough curve. For sorbing tracers, being strongly influenced by matrix diffusion, $\tau_0$ is the most significant parameter.	a. The impact of certain parameters may be different in the flow model to that in the transport model. The transmissivity of the Feature A significantly influences the flow model (drawdown), but the influence on the transport model is small, since the flow in the Feature was given. Skin factor used to decrease the conductance of the channels close to the tunnel, influence both the flow and transport.	<b>4E</b> The variance of the transmissivity field and the ratio between the hydraulic and transport apertures seemed to be coupled. To explain both the drawdown and the transport time a larger transmissivity variance was needed than was possible to use for numerical reasons. In the present model the most important parameter is the ratio between hydraulic and transport apertures. <b>4F</b> Groundwater transit time, sorption parameters and geometry of the transport channel. Tracer test seemed to be dominated by the advective flow field and groundwater transit time is important. The number and widths of the parallel flow channels together with the sorption parameters are important for tracer interaction.	The flow geometry and the hydraulic conductivity were the most significant because they determined the tracer transport path and time in the experimental area. For the sorbed tracers, another significant parameter is $K_d$ , which affects not only the transport time but also the maximum concentration of the tracer.	d) The matrix diffusion and sorption parameter ( $k$ ) most significant.

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<b>e Compare the calibrated model parameters with the initial base, comments</b>	The calibrated transmissivity at KXTT3 R2 is much larger than in the initial database. The large drawdown at KXTT3 R2 during the tracer tests cannot be explained by the transmissivity in the initial database. The calibrated matrix sorption coefficients are 4–19 times the initial data. The calibrated surface sorption coefficients are 0.56–8 times the initial values calculated from $K_d$ data for the 2–4 mm fraction after 1 day.	The flow properties of feature A are similar to those assumed in the hydraulic characterization. The transport pathway geometry is based on the DFN model for the fracture network containing Feature A. The immobile zone properties from calibration are consistent with microstructure data.	The only two transport parameters which can be compared with laboratory data are the pore diffusion coefficient and the distribution coefficient $K_d$ . By inverse modelling of the STT1 tracer test, in-situ values (best-fit) values could be extracted. Within a factor of five these best-fit values were always consistent with measured laboratory measurements and were used for the predictions of the STT2 tracer test.	In general, no large differences are found between the model used in the prediction of the earlier tracer tests and the model used for prediction of the STT2. No conditioning of the transmissivity at the injection or extraction locations are performed.	<b>4E</b> Calibration indicated larger variance of T-field than estimated in structural model. Understandable since estimate in structural model based only on hydraulic information. <b>4F</b> Interaction with the surrounding of the advective flow field has been stronger that was estimated based on the laboratory data of the sorption and diffusion properties.	The model parameters (distribution of fracture conductivity, fracture aperture, dispersion length, and effective porosity) calibrated in 4C/4D were not significantly changed in 4E and 4F. Hence, the model used for 4E/4F is compatible with the model used for 4C/4D.	See the TRUE-1 Final Report by Winberg et al., (2000).
<b>7 Sensitivity analysis</b>							
<b>Identify the sensitivity in your model output to:</b>	Not sensitive to discretisation due to small elements near borehole.	The transport model using Laplace Transform Galerkin internally discretizes the pipes to ensure mathematical stability. This is transparent to the user, and the results are insensitive to any discretization specified for the pipe network.	In the flow model 10 streamtubes were represented by a single streamtube due to the very narrow experimental flow field. Hence, velocity variations between the streamlines are of minor importance. The underlying transmissivity field was considered to be homogeneous. No discretisation scheme was used in the transport part of the model.	The channel size was maintained constant in the predictions. In preliminary simulations was found that the results are only slightly influenced by the discretisation if channels shorter than 1.0 m were used.	<b>4E</b> Resulting dispersion depends to some extent on discretization. <b>4F</b> Not relevant	Two meshes were used for Task 4C/4D to identify the sensitivity of the model to the discretisation of the finite element grid.	Did not test (tested in Tasks 4C and 4D).
<b>a) The discretisation used</b>							
<b>b) The transmissivity (distribution) used</b>	We did not perform any sensitivity analyses to the transmissivity.	The flow field is dependent directly on the transmissivity of both Feature A and the intersecting background fractures. However, the transmissivity distributions used arise directly from the data, and were therefore not studies as sensitivity parameters.	Only one referenced value for the fracture conductivity $K_f$ (HRL 97-13, p.7) was used. However, the sensitivity of such a value was not investigated.	The mean value of the transmissivity distribution varied in order to match the drawdown in the injection and extraction sections. In some cases, the standard deviation of the transmissivity was varied to fit the dispersion of the tracers. The transport of the tracer is largely uninfluenced by the transmissivity of Feature A, since the flow rate into the extraction section is given.	<b>4E</b> Mean transmissivity may have strong influence on recovery because of the background head field. Applied correlation length not so important. <b>4F</b> Not relevant	The hydraulic conductivity and fracture aperture have been varied.	Did not test (tested in Tasks 4C and 4D).
<b>c Sensitivity to transport parameters</b>	Aperture, dispersivity and surface related sorption coefficient in Feature A. Dispersivity and sorption coefficient in the rock matrix. Our model output is very sensitive to the aperture of Feature A and the sorption coefficient in the rock matrix	Advective velocity scales directly with transport aperture. Immobile zone and surface sorption depend directly on the immobile zone transport properties of thickness, porosity, and reactive surface area.	This item was not investigated. The analysis of both tracer tests showed that the (longitudinal) dispersivity only plays a minor role and is a suitable quantity only for a certain fine-tuning of the tracer breakthrough curve. Pecllet numbers between 20 and 40 do not essentially modify a given breakthrough curve.	The flow porosity or the volume of the channels is directly correlated with the residence time. The model shows a low sensitivity to the values used for the effective diffusion and sorption constants, since these effects are small for the most of the tracers. The only tracer that shows a significant sorption is caesium	<b>4E</b> The fitted ratio between the hydraulic and transport apertures controls the mean breakthrough time. <b>4F</b> Sorption, diffusion and porosity properties of the rock as well as channel geometry have direct influence on the breakthrough.	Transport parameters, e.g. flow porosity, dispersivity and diffusion coefficient were also checked to determine their influence on transport. In Task 4E, the sensitivity of the $K_d$ value and the error in the measurement of the breakthrough curve have been studied.	The following parameters Water residence distribution $g(t)$ , Enhanced diffusion factor $f$ , Surface sorption coefficient $K_a$ , $\beta$ and $\tau$ relationship, Sorption in the gouge material $K_a$ , input function

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<b>8 Lessons learned</b> Given your experience in implementing and modelling the TRUE-1 site, what changes do you recommend with regards to: a1 to experimental site characterisation	Measurement of the spatial distribution of aperture in a fracture by a resin injection experiment	1) Increase emphasis on fracture microstructure and geological information 2) Better control of tracer injection 3) Increased use of high resolution flow logs to characterize all conductive fractures and their connectivity influencing the experiment		The experimental site characterisation is sufficient to predict tracer tests with non-sorbing species on the detail scale..	Flow rate measurements to estimate the sensitivity of the test arrangement to the disturbances in the injection or background flow field. Sorption properties of the tested fracture as well as the fracture filling materials need to be known.	The experimental site of TRUE was very good characterised.	No comments.
<b>a2 Recommended changes to experimental design</b>	Dipole tracer tests in both forward and reverse directions between two boreholes	1) Increase the time period for tracer experiments, so that the tail of every tracer transport curve is essentially completed. 2) Increase the monitoring for tracer pathways other than those to the primary sink.	The experiments are well conducted, very stimulating and interesting. An important weak point of the experiments, however, is the injection device which hides with its long injection tail important information on nuclide rock interaction.	The injection technique could be improved. Most of the tracers enters Feature A after the short active injection period. Therefore a reduction of the amount of residual tracer would be beneficial. Also, the mass of injected tracer is difficult to determine. Another aspect is the choice of tracers for the tests. Most of the sorbing tracers show a very low sorption, therefore the transport is mainly controlled by the flow porosity, which has small or negligible impact in the transport of radionuclides under repository conditions. The tracer tests using Caesium is the only test with valuable information.	The short lasting source term needs well developed techniques for the sampling of the source terms and injection flow rate.	Concerning the double peak in the input function, the injection technique should be improved.	No comments.
<b>a3 Recommended changes to presentation of characterisation data</b>	We do not have any suggestion.	Increase emphasis on geological and microstructural data.	It is highly appreciated to perform calculations using a Dirac delta-input in order to compare the results of different models. However, they should be made in the analysis of a tracer test rather than for the predictions.	The presentation of the characterisation data was adequate.	Emphasis on transient behaviour of transport (following the decay of the source term tailing is of no interest).		No comments.
<b>a4 Recommended changes to performance measures and presentation formats</b>	We think that the peak and the peak time are the more important performance measures than the tracer recovery or the tracer travel time, t50.	Treat mass recovery and the shape of the breakthrough curve separately. Therefore breakthrough curves should be presented as normalized by mass recovery, and percent mass recovery during the experiment) should be treated as an importance performance measure.	With the finally accepted presentation format which considers tracer flow normalised to total injected mass a consistent intercomparison between different nuclides but also between different models can be made. Values for the total injected tracer masses as well as for the injection flow rate should be delivered to avoid unnecessary discrepancies between models and experiments.	Regarding performance measures and presentation formats; they are sufficient as they are.	Performance measure for the very high recovery i.e. t95 does not necessarily describe the spread of the breakthrough curve but it might include also a great deal of numerical uncertainty. Different models should be compared using breakthrough curves calculated for the dirac source term.	The recovered mass should be evaluated with respect to the initial mass as a performance measure.	No comments.

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<b>b</b> What additional site specific data would be required to make a more reliable prediction of the tracer experiments?	The spatial distribution of aperture in Feature A	Microstructural information (such as flow wetted surface), diffusivities of gouge materials and altered rim zone, and geochemistry of minerals within Feature A and other fractures forming transport pathways.	Information on structural geology on the mm to cm scale helps refining a given model and provides limits for transport parameters.	Better knowledge of the boundary conditions, hydraulic head at different locations in the rock mass during the time when the experiment is carried out.	Sorption properties of the tracers in the tested feature. This means that also the structure of the fracture needs to be known. In this kind of experiment the detailed characteristics of the advective flow field is important. However, the advective flow field can never be characterised in the detailed scale needed.	The additional measurement of the concentration in the other boreholes and/or in the packer interval in Feature B would provide more detailed information about the tracer distribution in the fracture system.	Parameters for sorption in the gauge material. Distribution of mineralogy along flow paths.
<b>c</b> What conclusions can be made regarding your conceptual model utilised for the exercise?	We have used two models for Task 4. One is a two-dimensional fracture model and another one is a three-dimensional model including the rock matrix. We have concluded that we need to use not the two-dimensional fracture model but the three-dimensional model in order to predict the migration of sorbing tracers even on a detailed scale.	The conceptual model utilized by our team was adequate for predicting Task 4E and 4F. However, the model does not address the longer term immobile zone porosities necessary for extrapolation to PA time and distance scales need to be added to the conceptual model	Presently we are working on the synthesis of all three tracer tests. Hence, final model parameter values will be specified later in the comprehensive modelling report.	See tables below.	<b>4E</b> Predictions of the sorbing tracers are systematically underestimating the breakthrough times. Taking into account the rather large pumping flow rates in the 4E tests it is not very likely that underestimation of the matrix diffusion is causing this. More probably the surface sorption in the feature A is not following the laboratory data used in the modelling. <b>4F</b> It is a reasonable concept to explain the transport processes. Parameters are based on the basic physical processes and no "lumped" parameters like hydro-dynamic dispersion are used.	Feature A can be considered as a planar fracture system using our conceptual model. But a channeling effect may exist and it could be described as a one-dimensional element in a two-dimensional model.	
<b>d</b> What additional generic research results are required to improve the ability to carry out predictive modelling of transport experiments on the detailed scale?	Measurement of the spatial distribution of aperture in a fracture by a resin injection experiment	Immobile zone properties and fracture microstructure are only beginning to be addressed and should be the focus for future generic research.	See 9c.	Research to obtain information about the flow wetted surface, and how this entity is correlated with the water flow rate.	<b>4E</b> The Darcy velocity field has to be solved either theoretically or experimentally in the scale of cm's in the transport path region before any sensible transport predictions can be made. <b>4F</b> Source term is very important. The behaviour of tracers and bypassing groundwater flow has to be known during the injection procedure.	On the site scale, complementary geoscientific methods, e.g., radar tomography, can be used to detect the distribution of tracer concentration during the tracer test so that it could be used as additional information for the modeller.	d) Improving the model for non-reactive tracers and obtaining more understanding of the $\beta$ - $\tau$ relationship.
<b>9 Resolutions of</b>	<b>issues and uncertainties</b>	The successful modeling of these experiments with homogeneous/effective flow and transport properties tends to support the use of such approaches. It is extremely important to address the fracture network and multiple pathway effects rather than assuming single confined aquifer solutions are directly applicable	Due to very rigid experimental conditions for the tracer migration experiments, i.e. the very high pumping flow rate at the extraction bore hole and nearly a passive injection, the hydraulic aspects and the heterogeneities on the dm scale play only a very minor role. Hence the flow and transport problem is predominantly reduced to a transport problem only. However, our model must be calibrated by independent experiments using conservative tracers in the same flow field. Further inferences with regard to the structural-hydraulic model on the block and detailed scale cannot be drawn.	CHAN3D may resolve fluid and solute transport occurring in channels or fractures. It includes advection in the channels and interaction with the rock matrix. For sorbing tracers, sorption within the matrix was included in addition to diffusion into the rock matrix. The model has been tested over different scales, from several hundreds of metres in LPT2, down to tens of metres in these predictions.	<b>4E</b> It is reasonable to model the feature A as hydraulically rather isolated two dimensional object. In the transport behaviour it seems reasonable to assume a single transport path. <b>4F</b> In this application no special inferences from the structural-hydraulic model are needed. Maybe the likely existence of the fault gauge in the feature A is such inference, but that information is applied more in the evaluation of the tracer test results than in the blind predictions.	In the fracture system Feature A, which was quite well-known, the tracer tests were interpreted by numerical modelling. The geological model and the numerical model were proved to be reliable.	Same model applies as in the predictions of the Dipole experiments (Task 4D).
<b>a</b> What inferences did you make regarding the descriptive structural hydraulic model on the block and detailed scale for the TRUE-1 site?	We infer that Feature A is highly heterogeneous in regard to transmissivity. Feature A is estimated to be highly transmissive in the vicinity of KXTT3 R2..						

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<p><b>b What issues did your model application resolve?</b></p>	<p>We used two models for the two-dimensional single fracture model. And the second one is a three dimensional model including the rock matrix. We could reproduce the breakthrough curves of the sorbing tracers not by two-dimensional model but by three-dimensional model. So we understood that the rock matrix significantly influences on migration of sorbing tracers on a detailed scale in crystalline rock.</p>	<p>1) The need for fracture network modeling to address transport pathways 2) The need for characterization of immobile zones and fracture microstructure 3) The importance of 3D hydraulic analysis to understand the flow field behind transport experiments 4) The usefulness of the type of effective transport properties used by this team and also by most PA modeling.</p>	<p>Although the model is rather simple it was able to predict relatively well the time-history of all applied tracers for all tracer tests. Only for Co, where no supporting laboratory measurements of transport parameters were available, and for Cs, enhanced differences between the predictions and the measurements could be observed. By a simple adjustment of some transport parameters a reasonable agreement for these two tracers could also be obtained. By fitting conservative tracer breakthrough data for calibration purposes important information about the behaviour of sorbing tracers could be deduced. In addition, the analysis of the field tracer tests showed strong coupling of sorption and matrix diffusion.</p>	<p>See above</p>	<p><b>4E</b> Mean transport aperture (which was actually already calibrated) and the spread of different transit times. Also, the coupling between the diffusion into the matrix and the flow field with the tested boundary conditions. <b>4F</b> It tries to answer to the question that are the basic physical processes of advection and molecular diffusion in the advective field and into the stagnant zones, fault gouge or rock matrix (together with sorption) able to explain the breakthrough curves.</p>	<p>The tracer transport parameter values (effective porosity, dispersivity, diffusion coefficient, and distribution effect) were determined by the modelling of the tracer tests under different test configurations. The Rockflow numerical models (flow model and transport model) have been tested for their applicability and suitability for a single-fracture system at the site scale (&lt; 10 m).</p>	<p>Effect of different mass transfer processes on the measured breakthrough.</p>
<p><b>c What additional issues were raised by the model application?</b></p>	<p>Our calibrated sorption coefficients are very different from the values obtained by the indoor experiments the initial database. So we think that it is a very important problem how we can estimate sorption coefficients accurately from indoor experiments.</p>	<p>1) The need for laboratory experiments to produce more directly applicable sorption coefficients 2) The increased importance of minerals, gouge, and breccia within fractures for transport, particularly when compared to the importance of aperture distributions which neglect internal structure (such as those obtained by resin methods).</p>	<p>From the analysis of the STT1b and STT2 tracer tests we conclude that the transport model is not capable to successfully model finer details of the trailing edge, especially for the sorbing tracers, and with consistent parameter values for all ten tracers. This is considered to be an indication of an additional transport mechanism, e.g., further porous zones accessible to matrix diffusion or an increased value for the specific interface area fracture/matrix. So far, no investigations in the frame of a "multiple rate diffusion model" have been made.</p>	<p>The impact of surface sorption was also studied in some simulations by using CHAN3D.</p>	<p>Comparing modelling results with experiments cannot uniquely distinguish between various concepts and modelling assumptions. Iterative cycles of experiments and modelling is required to test critically model performance. The influences of the injection procedure to the breakthrough curves might have important role in the interpretation of the breakthrough curves.</p>	<p>The question is whether the model and parameters can be scaled up. Extrapolation of the results from site scale to large scale should be investigated in the next step.</p>	<p>The need for improving the model for non-reactive transport, additional analyses of the impact of the <math>\beta</math>-<math>\tau</math> relationship</p>