Technical Report

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Evaluation of modelling of the TRUE-1 radially converging and dipole tests with conservative tracers

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

Tasks 4C and 4D

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May 1999

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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 4C and 4D is evaluated, which comprised predictive modelling of the radially converging tracer tests (RC-1) and dipole tracer tests (DP-1 – DP-4) performed within the TRUE-1 tests using non-sorbing tracers. The tests were performed between packed off boreholes penetrating a water-conducting geological feature with a simple structure (Feature A). These tests are to a great extent preparatory steps for the subsequent tests with sorbing radioactive tracers (STT-1, STT-1b and STT-2). In Tasks 4E and 4F of the Äspö Modelling Task Force predictive modelling of the sorbing tracer tests is performed.

Eight modelling teams representing seven organisations have performed predictive modelling using different modelling approaches and models. The modelling groups were initially given data from the site characterisation and data on the experimental set-up of the tracer tests. Based on this information, model predictions were performed of drawdown, tracer mass recovery and tracer breakthrough.

The performed predictions shows that the concept of Feature A as a singular well-connected feature with limited connectivity to its surroundings is quite adequate for predictions of drawdown in boreholes and conservative tracer breakthrough. Reasonable estimates were obtained using relatively simple models. However, more elaborate models with calibration or conditioning of transmissivities and transport apertures are required for more accurate predictions.

The general flow and transport processes are well understood, but the methodology to derive the necessary parameters for predictions needs development. The present understanding of the heterogeneity of the feature is limited and needs to be further evaluated. An issue that came in focus in this study is how to find a suitable relationship between the hydraulic fracture aperture derived from the hydrological tests and transport aperture derived from the tracer experiments. Furthermore, the use of extrapolation in assigning the boundary conditions used in the modelling gave rise to some uncertainty in the flow conditions in the outer parts of the feature.

The performed tracer experiments and the modelling work have increased the understanding of the groundwater flow in Feature A and have contributed valuable knowledge and experience for the subsequent more elaborate experiments within TRUE-1, e.g. the tests with sorbing tracers. The continued experimental work within TRUE-1 and the continued modelling work within Task 4 shows that a sufficient understanding has been obtained of at least the upstream part of the structure.

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 4C and 4D is evaluated. These tasks comprised predictive modelling of the radially converging tracer tests and dipole tracer tests performed within the TRUE-1 tests using non-sorbing tracers. These tests were performed between packed off boreholes penetrating a water-conducting geological feature with a simple structure (Feature A). The tasks are to a great extent preparatory steps for Tasks 4E and 4F, which comprise predictive modelling of tracer tests performed with a collection of sorbing, slightly sorbing and non-sorbing tracers.

A total of eight modelling teams representing seven organisations have performed predictive modelling using different modelling approaches and models. The modelling groups were initially given data from the site characterisation and data on the experimental set-up of the tracer test. Based on this information, model predictions were performed 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 majority of models describe Feature A as a two dimensional planar fracture. Both homogeneous and heterogeneous models have been used with different approaches for assigning the properties of the fracture. For the heterogeneous models both deterministic

and stochastic representations have been used. In a varying degree have fractures connecting to Feature A been considered in the models, for example through the use of discrete fracture network models and channel network models.

The performed predictions show that the concept of Feature A as a singular well-connected feature with limited connectivity to its surroundings is quite adequate for predictions of drawdown in boreholes and conservative tracer breakthrough. Reasonable estimates were obtained using relatively simple models. However, more elaborate models with calibration or conditioning of transmissivities and transport apertures are required for more accurate predictions. The modelling work performed within these tasks also demonstrate the benefits of using several models based on different concepts and of varying complexity for predictions and evaluations.

The general flow and transport processes are well understood, but the present understanding of the heterogeneity of the feature is limited and needs to be further evaluated. Measurements of the spatial aperture distribution by injection of resin are planned after the tracer tests have been completed. An additional issue that came in focus in this study is how to find a suitable relationship between the fracture aperture derived from the hydrological tests (hydraulic aperture) and that derived from the tracer experiments (transport aperture or mass balance aperture). This is essential in order to correctly predict both drawdown and tracer breakthrough. The modelling teams have dealt with this by independent calibration of a transport aperture or by introducing scaling relationships between transmissivity and transport aperture. However, such relationships are likely to be very site specific and their generality and use for predictive purposes needs to be further evaluated.

The boundary conditions used in the modelling have generally been assigned by extrapolation of the measured heads in the boreholes. This gave rise to some uncertainty in the flow conditions in the outer parts of the feature.

The methodology to derive the necessary parameters for predictions needs development. The tracer tests were preceded by a site characterisation, including hydrological tests and a preliminary tracer experiment. However, the modelling teams have not used the data set from the site characterisation to its full extent for their predictive models (e.g. the interference tests and pressure build-up tests). This indicates a need for development of methods to make use of all data produced from the site characterisation in the modelling. The conditioning of the transmissivity field on measured transmissivites and heads seems to be a promising methodology.

The performed tracer experiments and the modelling work have increased the understanding of the groundwater flow in Feature A and have contributed valuable knowledge and experience for the subsequent more elaborate experiments within TRUE-1, e.g. the tests with sorbing tracers. Predictive modelling of the tracer tests with sorbing tracers is performed within Tasks 4E and 4F. The subsequent experimental work within TRUE-1 and modelling work within Task 4 shows that a sufficient understanding has been obtained of at least the upstream part of Feature A characterised by boreholes KXTT3, KXTT1 and KXTT4.

Contents

List of Figures

List of Tables

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 correctly 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) have the objectives to conceptualise and parametrise an experimental site using both conservative and sorbing tracers in a simple test geometry, and to improve methodologies for tracer tests on a detailed scale (Winberg, 1994). Additional experiments performed within this stage of TRUE concerns the injection of resin in fractures for obtaining aperture distributions, and testing sampling and analysis technologies for evaluating matrix diffusion. The work performed within TRUE-1 is to a large extent a learning exercise contributing data and experiences for the future more elaborate tracer tests that will be performed within the TRUE 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. 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 (Task 4C) and dipole tracer tests (Task 4D) performed within

TRUE-1 using non-sorbing tracers. These tests were performed between packed off boreholes penetrating a water-conducting geological feature with a simple structure. The tracer tests were preceded by a characterisation of the site and a preliminary tracer experiment. A total of eight modelling teams representing seven organisations have performed predictive modelling using different modelling approaches and models. The modelling groups were initially given data from the site characterisation and data on the experimental set-up of the tracer experiment. Based on that, model predictions were performed. 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 and the modelling are compiled in Ström et al. (1996 and 1997). The work performed by the modelling groups is reported in International Cooperation Reports (ICR-reports), see Table 1-1.

Table 1-1 Organisations and modelling teams participating in Tasks 4C and 4D

Organisation	Modelling team	Representative	Task 4C	Task 4D	Reference
CRIEPI	CRIEPI	Y Tanaka	X	X	ICR 97-07
PNC	Golder Associates	W Dershowitz	X	X	ICR in prep.
SKB	KTH-CHE	L Moreno	X	X	ICR 98-01
POSIVA	VTT Energy	A Poteri	X	X	ICR 98-03
BMBF	BGR	L Liedtke	X	X	ICR 98-02
SKB	KTH-TRUE	J-O Selroos	X	X	ICR 98-07
ANDRA	CEA-DMT	E Mouche	X		
UK Nirex	AEA Technology	D Holton	X		ICR 98-06

This evaluation report focuses on the lessons learned from the modelling work in terms of 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 largely based on answers to the questionnaire sent out to the modelling teams. The discussion focuses on how processes and features are described in the models, the calibration made against previous experiments and the sensitivity studies performed. The chapter also discusses lessons learned and remaining unresolved issues. In Chapter 6 the main conclusions of the Modelling Task 4C and 4D are given. The appendices include data distributed to the modelling groups, the executive summaries provided by the modelling groups and also a compilation of the answers to the questionnaire for Tasks 4C and 4D.

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 preinvestigations and site characterisation started in 1986. Excavation of the underground facility started in October 1990 and was completed in June 1995. 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. The underground excavations are connected to the Äspö Research Village by a hoist shaft and two ventilation shafts.

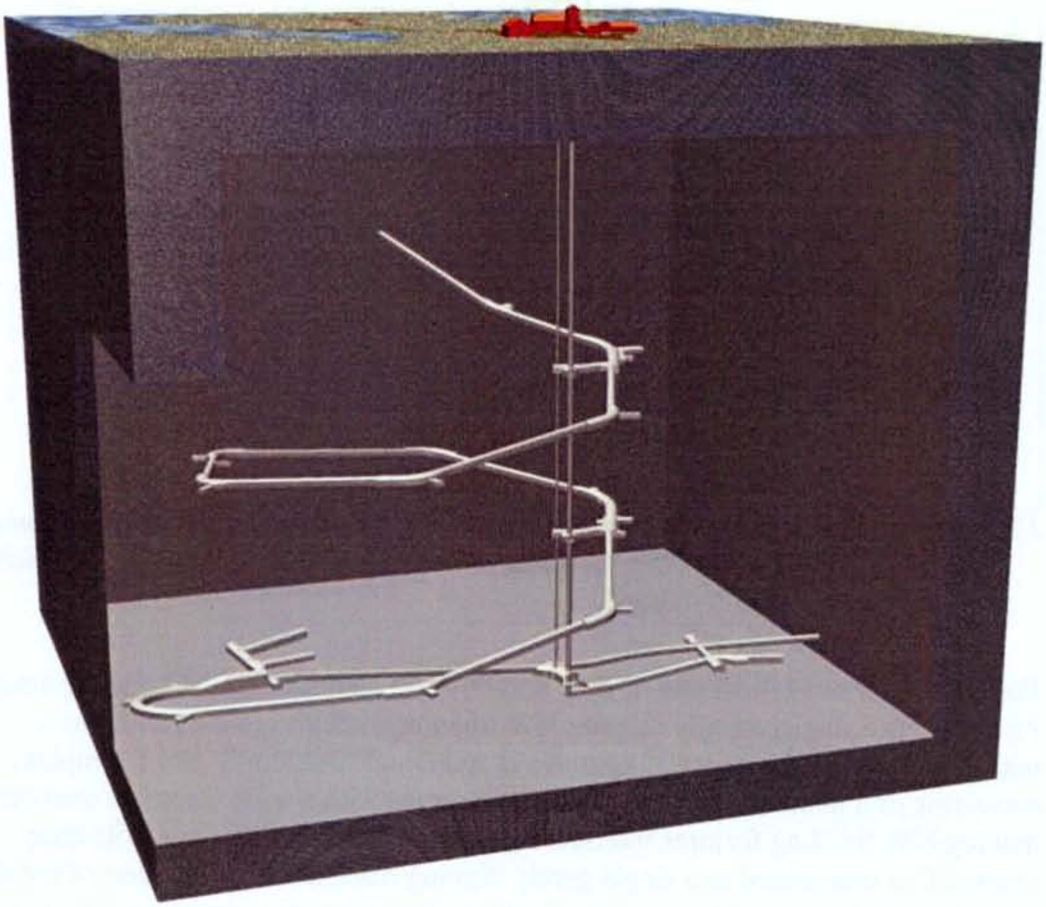

Figure 2-1 General layout of the Äspö HRL.

Äspö tunnel and TRUE niche

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.

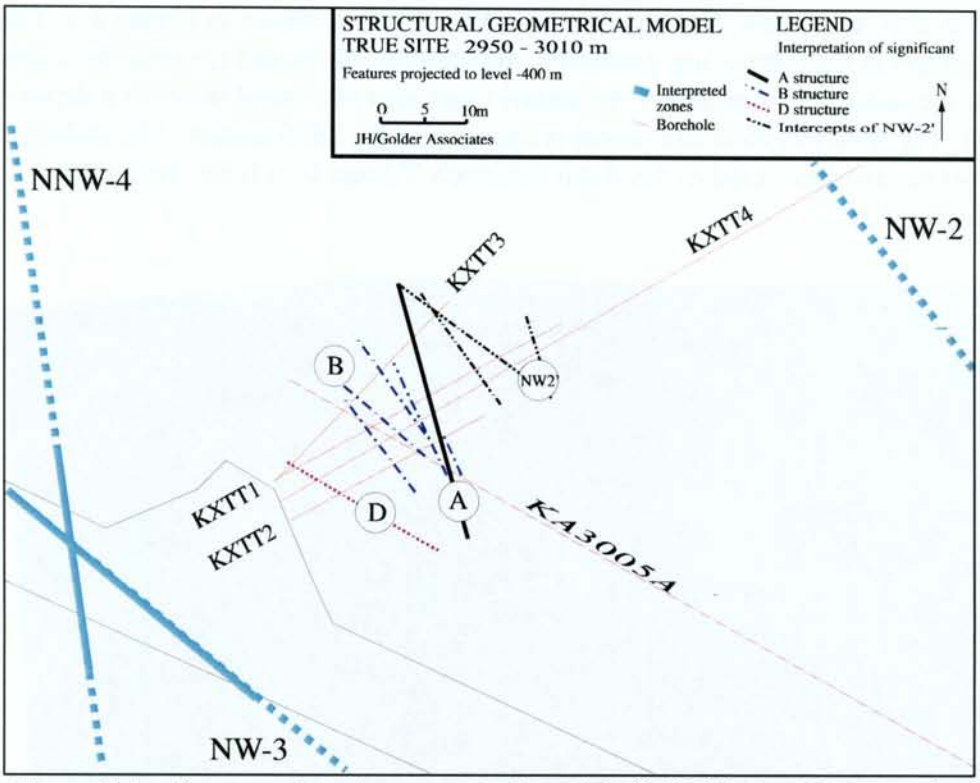

Figure 2-2 Structural and geometrical model of TRUE site. Horizontal section at Z=-400 m showing bounding minor fracture zones and features identified in the TRUE-1 Block.

Four minor features (Features A, B, C and D) were identified in the borehole array. Feature A is a single, 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. The extension of the feature is not known, but it could potentially facilitate the hydraulic connection between Features A and B.

In the Preliminary Tracer Test (PTT) two short-term tracer tests were performed in Feature A and in the nearby Feature B. The purpose of the tests was to test the injection and sampling equipment, and to obtain preliminary estimates of the transport parameters. After the completion of the preliminary tracer tests Feature A was selected as target feature for the further experiments.

The preliminary tracer test in Feature A was conducted as a radially converging test between the borehole sections KXTT1 P2 and KXTT3 P2 (distance approximately 5 meters) using a pumping rate of 0.87 l/min in KXTT3. The tested flow path was shown to have a good connectivity and yielded a high tracer recovery. However, the preliminary test was a short-term test performed under a high gradient, which resulted in very short travel times (of the same magnitude as in the testing equipment). The transport parameters that were determined from this test are therefore only rough estimates.

2.2 Radially converging tracer tests (Task 4C)

2.2.1 Objectives

The objectives of the TRUE-1 Radially Converging Tracer test No1 (RC-1) were to determine the transport parameters (flow porosity, dispersivity and fracture conductivity) and to test the connectivity of the selected hydraulic feature (Feature A). The experiment was also made to test techniques, tracers and equipment for injection and sampling of tracers in low transmissivity rocks for future stages of the TRUE project.

2.2.2 Definition and set up

The test was performed in a radially converging flow geometry with pumping in one borehole section and injection of tracer in four borehole sections penetrating Feature A (Andersson et al, 1996). A reinstrumentation of the boreholes was made prior to the test in order to optimise the location of the borehole sections. Pumping was performed in the new borehole section KXTT3 R2 and tracer was injected in the borehole sections KXTT1 R2, KXTT4 R3, KXTT2 R2 and KA3005 R3, see Figure 2.3. The travel distances ranged from 4.7 to 9.6 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 reducers (dummies). Two tracers, a fluorescent dye and a metal complex, were injected in each section with an initial mixing period of about 11 minutes. Thereafter, the tracer concentration in the injection section decreased slowly due to the induced flow by pumping in section KXTT3 R2. The tracer injection can be described as a decaying pulse. Due to the low flow rates and the relatively large volumes of the injection sections the decay of the injection pulse was relatively slow. The time until the concentration reached half its original value ranged from about 150 hours to more than 500 hours.

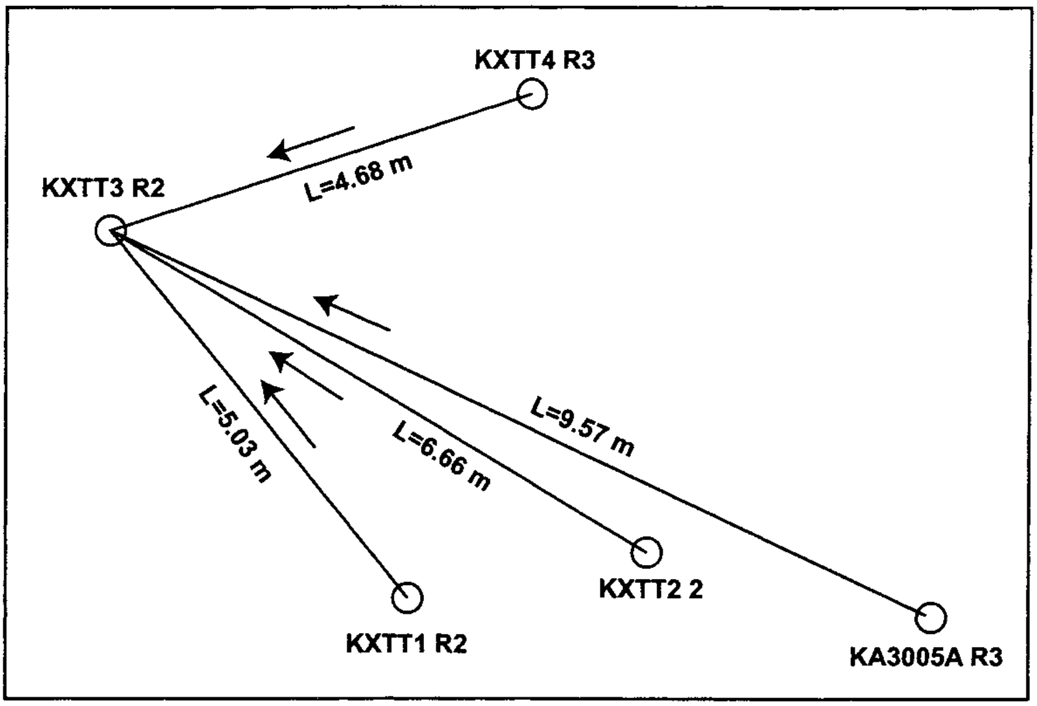

Figure 2-3 Test geometry and borehole intersection pattern with Feature A for the TRUE-1 Radially converging tracer test (RC-1).

Pumping in the withdrawal section (KXTT3 R2) at a rate of 0.2 l/min started six days prior to the injection in KXTT1 R2 and KXTT4 R3. The withdrawal section was sampled with an initial sampling frequency of one sample per 2 minutes gradually increasing to a sample per 6 hours after three weeks. A rapid breakthrough occurred from the injection sections KXTT1 R2 and KXTT4 R3, 5% of the recovered mass had arrived after 25.5 and 20.9 hours, respectively. Injection into the two remaining sections followed 14 days later. One day prior to the injection in the remaining sections a degassing was made of the injection section KXTT2 R2, which resulted in a permanent increase of the flow in the injection section KXTT1 R2. After two weeks of injection in KXTT2 R2 and KA3005 R3, no tracer had arrived at the withdrawal section. The withdrawal rate was then increased to 0.4 l/min, which resulted in a breakthrough from KXTT2 R2. A further increase of the withdrawal rate to about 3 l/min gave breakthrough also from section KA3005 R3.

2.2.3 Data base

Several deliveries of documents and data were made to the participating organisations and the modelling groups. Four deliveries made in February to April 1996 contained background structural-hydraulic information, data from preliminary tests performed at the TRUE-1 site and data on flow and injection concentrations for the radially converging tracer tests. The deliveries included:

- Final draft of report ”Descriptive structural-hydraulic models on block and detailed scales of the TRUE-1 site” (Winberg, 1996).
- Test design for the TRUE-1 radially converging tests RC-1 (part of Progress Report).

- Performance measures and presentations format.
- Data from the performed site characterisation, including:
  Borehole deviation data
  Pressure data from the pressure build-up tests
  Flow data from the pressure build-up tests
  Data from single packer flow logging
  Pressure data from the interference tests
  Drawdown and recovery data from the interference tests
  Data from preliminary tracer tests in Features A and B (injection concentration vs time, tracer breakthrough in the pump sections vs time).
- Complementary experimental data from RC-1. Information regarding pumping rate and injection concentration as a function of time.
- Some clarifications of the geometry of 3rd order zones NW-2 and NW-3.
- The final draft version of "Discrete fracture analysis in support of the Äspö Tracer Retention Understanding Experiment (TRUE-1)" (Dershowitz et al, 1996).

Finally the experimental results of the radially converging tests were distributed in October 1996, containing the following data:

- Injection concentration versus time of Uranine (KXTT1 R2), Rhodamine WT (KXTT2 R2), Amino G (KXTT4 R3), Eosin Y (KA3005A R3).
- Breakthrough data versus time for Uranine, Amino G, Rhodamine WT, Eosin
- Head data (metres above sea level) for KXTT1 R2, KXTT2 R2, KXTT2 R2, KXTT4 R3, KA3005A R3.
- Absolute pressure (kPa) for the borehole sections given above.
- Complete data set on pump flow rate and electrical conductivity as a function of time.

2.3 Dipole tracer tests (Task 4D)

2.3.1 Objectives

The objectives of the TRUE-1 dipole tests (DP1 – DP4) were firstly to test methodology and equipment for tracer tests in low transmissive fractures, and secondly to obtain results for intercomparison with the results of the previously performed preliminary tracer tests (PTT) and the radially converging test (RC-1). Furthermore, the dipole tests should increase the understanding of the properties of the target feature (Feature A) and how the boundary conditions affects solute transport in that feature.

2.3.2 Definition and set up

Four dipole tracer tests (Andersson et al., 1997) were performed between different borehole sections penetrating Feature A, see Figure 2-4. The geometry of the different dipole tests is given in Table 2-1.

Table 2-1 Geometry and flow rates in dipole tracer tests

Dipole test	Injection borehole	Injection rate (ml/min)	Extraction borehole	Extraction rate (ml/min)
DP-1	KXTT1 R2	10	KXTT3 R2	102
DP-2	KXTT2 R2	10	KXTT1 R2	36
DP-3	KXTT2 R2	3.5	KXTT1 R2	36
DP-4	KXTT2 R2	10	KXTT4 R3	52

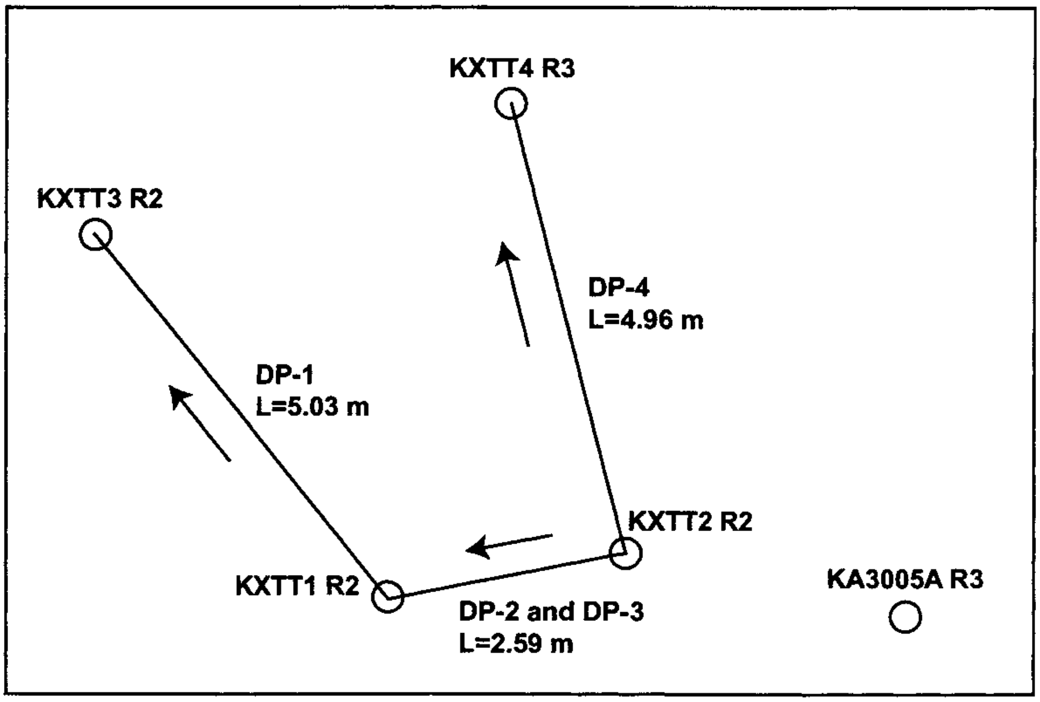

Figure 2-4 Test geometry and borehole intersection pattern with Feature A for the TRUE-1 Dipole test (DP1 - DP4).

The tracer injection was made using the same methodology as in the radially converging tracer tests, i.e. a decaying pulse injection. However, in the dipole tests the decay of the pulse was much faster due to the flow induced by the injection of unlabeled water in the injection sections. The time until the concentration in the injection section reached half its original value ranged from about 2 to 6 hours.

The withdrawal sections were sampled using the same methodology as in the radially converging tracer test. The initial sampling frequency was one sample every 5 min gradually increasing to one sample every hour. The injection sections were sampled by a constant leak in the circulation loop of the borehole fluid.

The hydraulic head in the borehole sections was measured before and during the test period.

2.3.3 Data base

A data delivery for the predictive modelling was sent out to the participating organisations and the modelling teams in November 1996. The delivery contained:

- Complementary information for the DP-1 – DP-4 tests. Pumping rate and the injection concentration as a function of time.
- Performance measures and presentation formats.
- Test design for the TRUE-1 dipole tests DP1-DP4 (part of Progress Report).

In a second data delivery in March 1997 the experimental results from the dipole tests DP-1 to DP-4 were distributed for use in the evaluation of Task 4D. The data comprised:

- Breakthrough concentration versus time in the extraction sections.
- Injection concentration versus time in the injection sections.
- Pump flow rate and electrical conductivity versus time for water pumped from the extraction holes.
- Hydraulic head versus time for KXTT1 R2, KXTT2 R2, KXTT3 R2, KXTT4 R3, KA3005A R3 during DP-1 – DP-4.

3 Modelling approaches

3.1 General approaches for modelling of groundwater flow and transport in fractured rock

Modelling of flow and transport in fractured rock has been an area of extensive research during the last decades. A major problem is how to adequately describe the heterogeneous nature of the flow paths in the rock with the available data and computing resources. The modelling work performed within Tasks 4C and 4D focussed on the flow and transport of non-sorbing tracers within a single feature on a scale of about 5 meters. Even at this scale heterogeneity may play an important role.

One model approach is to treat the fracture plane 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 have been 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 usually 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.

3.2 Approaches applied by the modelling teams

3.2.1 Introduction

A wide range of models and modelling approaches have been applied in Task 4C&D. In Tables 3-1 and 3-2 a summary is made of the flow and transport models used.

The majority of models describe Feature A as a two dimensional planar fracture. Both homogeneous and heterogeneous models have been used with different approaches for assigning the properties of the fracture. For the heterogeneous fractures both deterministic and stochastic representations have been used. In a varying degree have fractures connecting to Feature A been considered in the models. The PNC/Golder group has also used a discrete fracture network model to evaluate the effect of intersecting fractures on the flow and transport in Feature A. The SKB/KTH-ChE group has used a channel network model with discrete representation of Feature A, Feature B and the tunnel. The BMBF/BGR group performed studies of the influence of Feature B.

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 different versions of the flow equation, while the tracer transport are either based on the advection-dispersion equation or on particle tracking methods. The former has been used in connection with deterministic models and the latter in connection with the stochastic methods.

Table 3-1 Summary of the models for the flow

TOPIC	CRIEPI	PNC/Golder(II)	PNC/Golder (III)	SKB KTH-ChE	POSIVA/VTT	BMBF/BGR	SKB KTH-TRUE	Nirex/AEA	Andra
Type of model	Deterministic continuum model (Stochastic in predictive modeling)	Deterministic continuum model	Discrete fracture network model (DFN)	Channel network model	Stochastic continuum model	Deterministic continuum model	Stochastic continuum model	Stochastic continuum model	Analytical model
Process description	Water flow in heterogeneous 2D fracture.	Water flow in a homogeneous 2D fracture.	Water flow in discrete 3D fracture network.	Water flow in discrete 3D channel network.	Water flow in heterogeneous 2D fracture.	Water flow in heterogeneous 2D fracture.	Water flow in heterogeneous/ homogeneous 2D fracture.	Water flow in heterogeneous 2D fracture	Water flow in a heterogeneous 2D fracture
Geometric framework and parameters	Feature A modelled as single flat square with side lengths 30m.	Feature A modelled as single flat square with side lengths 48 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.	Modelling of feature A and B, tunnel with niche (A extended to boundaries, B treated as confined fracture) and channels in a rock block with size 30x30x40 m.	Feature A modelled as heterogeneous fracture plane,15x20 m for the radial test and 20x16 m for the dipole test .	Feature A modelled as a heterogeneous plane, 20x20 m. Feature B included but with negligible influence.	Feature A modelled as a heterogeneous plane (DP also homogeneous), 20x20m	Feature A modelled as a heterogeneous plane, 25x20 m	Feature A modelled as an infinite plane
Material properties and hydrological properties	Transmissivity	Transmissivity	Transmissivity storativity, aperture	Channel conductances	Transmissivity	Fracture conductivity	Transmissivity	transmissivity (log-norm Tr.->log-norm Ap.->log-norm Perm.)	Transmissivity Fracture aperture
Spatial assignment method	Lognormal transmissivity with correlation length of 1 m, estimated by kriging on transmissivities in boreholes from drawdown during tracer test.	Constant parameters based on results of preliminary tests used in simulation.	Background fracture: lognormally distributed size and transmissivity from analysis of flow logging in the TRUE-1 borehole array.	Lognormal conductances, uncorrelated in space. Not conditioned to measured boreholes transmissivities Reduced conductance in channels in contact with tunnel.	Lognormal transmissivity whith correlation length of 0.4 metres. Mean value from experimental data, SD from previous test. Not conditioned to measured boreholes transmissivities	Conductivity in fracture adjusted to minimise error in drawdown from previous tests.	Lognormal transmissivity with correlation length of 1 metre. Aperture from calibration against experimental arrival travel time from preliminary tracer test.	Lognormal transmissivity conditioned on the known values of the transmissivity using kriging	Constant parameters based on results of preliminary tests used in simulation.
Boundary conditions	All surrounding boundaries: fixed hydraulic heads. Injection sections: fluid flux estimated from decline of measured tracer concentration in injection holes.	Hydrostatic, constant head on the boundaries. Local head, conditions consistent with heads measured in boreholes before initiation of experiment	Fixed head boundary conditions on the six edges of the model and time varying flux in packer intervals for the 5 boreholes.	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. 4C:from measured natural head. 4D:zero head. Higher fixed transmissivity around borehole sections.	Fixed hydraulic head at top of feature A and at a point on north side to simulate natural flow conditions. Extraction/injection of water in test bore holes.	Head boundary conditions on all boundaries, extrapolated from boreholes. (Head values when no pumping)	No flow boundaries on top and bottom head boundary conditions on the other sides in variant A. Head boundary conditions on all sides in variant B2, B3, B4, B5	Infinite boundaries
Numerical tool	FEGM/FERM	SEEP/W	Fracman/MAFIC	CHAN3D-flow	TFIELD/FEFLOW	DURST/Rockflow SM2	Marflow	NAMMU	
Numerical method	Finite element method	Finite element method	Finite element method	Resistance network, preconditioned conjugated gradient method.	Finite element method	Finite-element method	Mixed hybrid finite element formulation	Finite element method	Analytical solution using the equation for radial flow
Output parameters	Hydraulic head, Darcy velocity	Hydraulic head	Hydraulic head, flow in fractures	Flow in channels, head in intersection points.	Head field and flow field.	Head field and flow field.	Head field and flow field.	Head field and flow field	Head differences between pumping/ injection boreholes.

Table 3-2 Summary of the models for the transport

TOPIC	CRIEPI	PNC/Golder(I)	PNC/Golder(II)	PNC/Golder (III)	SKB KTH-CE	POSIVA/VTT	BMBF/BGR	SKB KTH-TRUE	Nirex/AEA	Andra
Type of model	Determinsitic continuum model	Analytical model	Deterministic continuum model	Discrete fracture network model (DFN)	Channel network model	Stochastic continuum model	Deterministic continuum model	Stochastic continuum model	Stochastic continuum model	Linear stochastic model
Process description	Advection, longitudinal and transverse dispersion.	Advection-dispersion in radially converging homogeneous flow field in dual porosity medium.	Advection Longitudinal and transverse dispersion	Advection, dispersion	Advection and matrix diffusion, spreading due to transport in different channels.	Advection, spreading due to spatially variable velocity and molecular diffusion.	Advection, longitudinal and transverse dispersion, diffusion in fracture plane	Advection, spreading due to spatially variable velocity.	Advection, spreading due to Taylor dispersion	Advection, longitudinal dispersion
Geometric framework and parameters	Feature A modelled as single flat square with side lengths 30m.	Feature A modelled as infinite flat square	Feature A modelled as single flat square with side lengths 48 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.	Modelling of feature A and B, tunnel with niche (A extended to boundaries, B treated as confined fracture) and channels in a rock block with size 30x30x40 m.	Feature A modelled as heterogeneous fracture plane,15x20 m for the radial test and 20x16 m for the dipole test .	Feature A modelled as a heterogeneous plane, 20x20 m. Feature B included but with negligible influence.	Feature A modelled as a heterogeneous plane (DP also homogeneous), 20x20m	Fracture A modelled as a heterogeneous plane, 25x20 m.	Domain modelled as a cone defined by the pumping and injection boreholes.
Material properties	Fracture aperture Longitudinal dispersivity Transverse dispersivity 1/10 of longitudinal	Fracture aperture Fracture porosity, dispersivity, rock block diffusion parameters	Fracture aperture Dispersivity	Fracture aperture Dispersivity	Flow porosity (channel volume), rock matrix porosity, diffusivity and flow wetted surface.	Hydraulic aperture, ratio between hydraulic and transport aperture.	Fracture aperture Dispersivity Diffusion coefficient effective porosity	Transport aperture from calib. against exp. mean travel time in preliminary test	Fracture aperture, molecular diffusion coefficient	Fracture aperture Longitudinal dispersivity
Spatial assignment method	Estimated to minimise difference between calculated and measured breakthrough.	Constant parameters based on results of preliminary tests used in simulation.	Constant parameters based on results of preliminary tests used in simulation.	Transport apertures based on Doe Law with calibration to previous tracer tests	Channel volume derived from conductance using cubic law.	Hydraulic aperture derived from transmissivity using cubic law. Transport aperture by ratio.	Constant parameters in fracture.	Constant aperture in fracture.	Lognormally distributed fracture aperture	Concentration and mass flux standard deviation deduced from preliminary tracer tests.
Boundary conditions	No flux of tracer across boundaries. Injection sections: time-varying mass flux of tracers.	Constant tracer injection, Dirac pulse injection or top hat injection	Tracer injection flow rate and concentration.	Tracer injection rate	Tracer injection flow rate and concentration.	Pulse injection, breakthrough curves calculated by convoluting with measured injection curve.	Tracer injection flow rate and concentration.	Pulse injection, breakthrough curves calculated by convoluting with measured injection curve.	Upstream:Unit tracer concentration Downstream:Zero concentration	Imposed concentration at the injection borehole, dispersive flux equal to zero at the pumping borehole
Numerical tool	FEGM/FERM	Moench solution	CTRAN/W	Fracman/MAFIC	CHAN3D-transport	BTSIMU	DURST/Rockflow TM2	Particle track. method	NAMMU	CASTEM2000
Numerical method	Finite element method	Laplace transform solution.	Finite element method	Particle tracking	Particle-following technique	Particle tracking method	Finite element method	Particle tracking method	Finite element method	Mixed hybrid finite element method
Output parameters	Concentration of tracers, breakthrough curves.	Breakthrough curves	Breakthrough curves	Breakthrough curves	Residence time distribution, breakthrough curves, particle trace.	Breakthrough curves	Breakthrough curves Concentration distribution	Breakthrough curves	Breakthrough curves pathlines	Breakthrough curves, mean and standard deviation

3.2.2 CRIEPI

The Central Research Institute of Electric Power Industry (CRIEPI) of Japan participated in Tasks 4C and 4D with the specific modelling objective of evaluating how a simple model could describe flow and transport in a heterogeneous fracture consistently with experimental results. The modelling group performed predictive modelling of Task 4C (Tanaka et al., 1996) and Task 4D (Tanaka et al., 1997a). After the experimental results were delivered also a fitting of their model to the results (Tanaka et al., 1997b).

Feature A was considered as an isolated fracture described as a flat square with a side of 30 m. The flow in the fracture is solved with the flow equation and the tracer transport using the advection-dispersion equation. Dispersion and diffusion in the fracture plane is taken into account, but no diffusion into the rock matrix. The calculations were made with a mesh refined in the central part where the boreholes were located. The number of elements in different simulations varied between about 1400 to 4000.

Radially converging test

In the predictive calculations of the radially converging test both a deterministic and a stochastic approach has been used. In the deterministic calculations the spatial distribution of transmissivity in Feature A was estimated by inverse analysis using the data from the interference tests. In the stochastic calculations the transmissivity was assumed to have lognormal distribution with parameters based on Winberg (1996) and a correlation length of 0.35 m. The transmissivity field was conditioned on the measured values in the boreholes. In the flow calculations the upper and lower sides of the modelled domain were assumed to be impermeable, while the subvertical sides were set at hydrostatic pressure. The transport calculations were performed with parameters derived from the preliminary tracer experiment. Time-varying mass flux of tracer was prescribed at the injection boreholes. The decline in tracer concentration in the injection section was estimated by an exponential function were the time constant was allowed to change with time.

Dipole test

Only the stochastic approach was used for the predictive modelling of the dipole tests. The borehole transmissivites were increased based on the measured drawdown in KXTT3. The adjusted transmissivities were used for the generation of the transmissivity field, but using the same standard deviation and correlation length as in the radially converging predictions. Two types of boundary conditions were used; in the first case by extrapolating the values at KXTT3 and KA3005A to the model boundaries, and in the second case by extrapolating the values at KXTT3 and KXTT2. The transport parameters assigned to the modelled feature were the same as in the radially converging predictions. In addition to modelling the injection with an exponential function the injection of a pulse was simulated by injection of a unit mass of tracer over 10 seconds.

Final calculations

In the final calculations, the transmissivity in Feature A was assumed to have a lognormal distribution with a spatial correlation length of 1 m. The spatial distribution of transmissivities in Feature A was estimated by kriging on the transmissivities of the borehole sections calculated from drawdown during the tracer tests. This gave a transmissivity field with large variation around the boreholes, but with an almost homogeneous field far from the boreholes. Secondly, the boundary conditions were determined from the hydraulic head field under natural conditions in the feature estimated from the measured heads in the boreholes. Separate head fields were used for the radially converging and dipole test due to the long term head changes. The fluid flux through the tracer injection sections was estimated from the injection concentration curves. The product of the fluid flux and the tracer concentration was used as the mass flux of injected tracer. In the simulations of the tracer transport the fracture aperture and the longitudinal dispersivity were calibrated to the results of the experiments. The best fit of the fracture aperture varied between 0.23 and 0.75 mm between the different tracer tests and the longitudinal dispersivity varied between 0.19 and 1.37 m.

3.2.3 PNC/Golder

The modelling team from the Power Reactor and Nuclear Fuel Development Corporation (PNC) of Japan and Golder Associates has participated in Tasks 4C and 4D with the purpose of improving the understanding of flow and transport in discrete fracture networks with the focus on transport and the role of fracture connectivity. Special issues addressed are the role of the head field in the modelling and the effect of intersecting fractures. The method used is to make predictions with different boundary conditions using both an analytical and a numerical two-dimensional continuum model (Dershowitz et al., 1996). The effect of intersecting fracture has been studied using a discrete fracture network model (DFN).

Four types of boundary conditions were studied:

- Hydrostatic: A constant head on all boundaries with gradients only due to the pumping.
- Point dilution: The difference in flow rate in the injection holes (derived from the rate of tracer dilution) is assumed caused by a hydraulic gradient over the test site.
- Local head: Boundary conditions consistent with local heads measured in the boreholes in Feature A before the experiment.
- TRUE-regional heads: Boundary conditions based on heads measured in all boreholes in the TRUE-1 block.

In the analytical and numerical models Feature A is treated as a two-dimensional homogenous fracture (confined aquifer). The analytical model describes transport in a double porosity medium with radially converging flow. For the dipole experiment a modified solution was used adding terms for the effects of the injection. The numerical model first solves the flow field, which is later used to calculate the transport using the advection-dispersion equation. The model has a capability to handle materials with heterogeneous properties, but was here only used for a homogeneous case.

The discrete fracture network model was used to describe a 50 x 50 x 50 m block containing a limited number of deterministic features (Feature A and in the dipole experiment additional features) in a stochastically generated network of fractures. The DFN model was considered to be of secondary importance for the predictive modelling, since a number of head measurements were available within the feature. Instead, the purpose of using it was to illustrate the behaviour of fracture networks.

The flow equation is solved for the network of fracture. Transport is modelled by particle tracking assuming complete mixing in fracture intersections. Dispersion is added by a stochastic component at each time step.

Radially converging test

The head fields obtained with the different boundary conditions were analysed to determine the possibility of recovery from the different injection points under the studied boundary conditions.

Calculations were made using the hydrostatic boundary condition for all models and using the local head boundary condition for the numerical continuum model. One realisation was made with the DFN model. The transmissivity, hydraulic conductivity and fracture aperture of Feature A were based on the evaluation of the preliminary tracer experiments (Dershowitz et al., 1996). The stochastic background features were generated based on data from Dershowitz et al. (1996) and data from analysis of the single-packer flow logging in the TRUE-1 borehole array (Winberg, 1996).

Dipole experiments

The PNC/Golder team used two concepts for the predictions of the dipole tests: small scale DFN modelling and analytical solutions. For the DFN-model, the large drawdown in KXTT2 observed in the radially converging test lead to the inclusion of a highly conductive pathway between KXTT2 and KXTT3. The radially converging test was simulated with a number of realisations of the stochastic fracture network. Predictions of the dipole test were made for the six realisations that gave a reasonable match to the observed drawdown and the observed breakthrough in the radially converging test. In the dipole simulations the boundary conditions were changed to account for the head changes that occurred between the experiments. Due to the small number of realisations the 5 and 95 percentile were calculated from the mean and standard deviation assuming a normal distribution.

The fracture aperture and longitudinal dispersivity used in the analytical continuum model for radially converging flow was calibrated on the results of the radially converging test. These parameters were then used in the model extended for dipole tests. The parameters calibrated from the KXTT1 injection were used for the dipole test with injection in KXTT1 and KXTT2 and the parameters calibrated from the KXTT4 injection were used in the dipole test with injection in KXTT4. No predictions of drawdown were made with the analytical model.

3.2.4 SKB/KTH-ChE

The Royal Institute of Technology/Department of Chemical Engineering (KTH-ChE) of Sweden on assignment of SKB has participated in Tasks 4C and 4D with the purpose of increasing the knowledge about important entities for flow and transport in fractured rock. Of particular interest was the possibility to study the effect of site geometry, boundary conditions and illustrate the effects of different transport mechanisms. An additional purpose was testing of the model CHAN3D by applying it to a specific experiment.

The modelling team has focussed on the flow and transport in a network of flow paths (channels) in the fractured rock volume (Gylling et al, 1998). The model is based on the concept that flow and transport takes 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 are described by a hydraulic conductance, assigned from a statistical distribution. The transport is 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 is 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 is 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 boreholes and Features A and B. The discrete features are 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 320000 channels.

A constant hydraulic head was assigned at the top, bottom and the vertical side away from the tunnel. The pressure in the tunnel was used as boundary condition on the opposite vertical side. The 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 Features A and B were assigned from measured transmissivities. No conditioning of the transmissivity was made at the intersecting boreholes. The mean transmissivity of the surrounding bedrock was calculated from the hydraulic conductivity of the rock mass. A lognormal standard deviation of 0.8 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 evaluations from the preliminary tracer test. 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 a lower flow porosity than those in the features. The specific flow wetted surface was estimated to be 1 m^2/m^3, which for a channel length of 0.7 m corresponding to a channel width of 0.25 m.

Radially converging tracer test

The head difference between the withdrawal and injection sections in the preliminary tracer test was used to calibrate the mean conductance in Feature A. The results showed that Feature A had to be extended to the model boundaries in order to give reasonable head differences. The volume of the channels included in Feature A was, in the case of prediction of the radially converging tests, determined from the flow porosity measured in the preliminary tracer tests.

Dipole tests

The mean conductance of the channels in Feature A was calibrated against the head difference between the withdrawal and injection sections in the radially converging tracer test. Also the volume of the channels included in Feature A was refined using the results of the radially converging tests.

Sensitivity studies

Simulations were performed with an increased transmissivity in Feature A in order to improve the match with the experimental drawdown in the radially converging tracer test. Furthermore, the conductance reduction for the channels connecting to the tunnel (skin factor) was varied in the range 10 - 30 to evaluate the effect of inflow to the tunnel.

3.2.5 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. Of special interest is the question of how the heterogeneity influences the flow rate distribution in the fracture plane and as a consequence of that, the interaction rate between transported solutes and the fracture walls in different parts of the fracture.

The team has modelled Feature A as a two-dimensional heterogeneous fracture plane using a stochastic continuum model (Poteri and Hautojärvi, 1998). No connecting fractures are included. The hydraulic head field in Feature A is calculated by solving the flow equation in two dimensions. The modelled plane had the dimensions 15 x 20 meters for the radially converging test and 20 x 16 m for the dipole test, which was judged to be large enough to have fixed head boundary conditions at the outer edges. The grid consisted of equally sized elements with a side of about 0.05 m for the radially converging test and about 0.1 m for the dipole tests. An isotropic transmissivity field was generated based on a lognormal transmissivity distribution and a spherical correlation function. The transmissivity field was not conditioned to the measured borehole transmissivities.

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 calibrated ratio between transport aperture and hydraulic aperture. Dispersion of the tracer due to hydrodynamic dispersion and molecular diffusion in the fracture plane was taken into account. Hydrodynamic dispersion was modelled explicitly by the heterogeneous flow field. Molecular diffusion was described by adding a random component to the particle displacement. The dispersion caused by matrix diffusion was estimated to be considerably smaller than that due to hydrodynamic dispersion and thus neglected. The breakthrough curves were calculated for a Dirac pulse injection. 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.

An alternative modelling approach was applied to some of the tracer tests, where the transport within individual channels is described. 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 is assumed to vary linearly from a maximum value at the centre to zero at the edges. The average concentration over the channel width is solved analytically.

Radially converging test

The transmissivity field used in predicting the radially converging tracer test was obtained by a simulation of the drawdown and transport times in the preliminary tracer test. The measured drawdown in the preliminary tracer test could be simulated using a lognormal distribution of the transmissivity with μ=-6.67 and σ=1.0. This is higher than the value calculated from the pressure build-up tests, but in the same magnitude as the value from the interference tests. The correlation length was set to 0.4 m based on the inferences made in the site characterisation report (Winberg, 1996). The transport time was found to be sensitive to the variance of the transmissivity field. Based on the head difference and the mean transport time in the preliminary tracer tests it was estimated that a suitable value for the standard deviation was σ=1.5 – 2 (Base $\log_{10}$). However, numerical difficulties excluded the use of a standard deviation exceeding 1. Correct transport times where therefore calculated using separate hydraulic and transport apertures. The local transport aperture was about 15 times larger that the hydraulic aperture. The transmissivity field was not conditioned on the measured borehole transmissivities. The part of the fracture closer than 0.2 metres to the pumping hole was assigned a high transmissivity value ($3\cdot10^{-3}$ m^2/s) in order to ensure a sufficient hydraulic conductivity between the boreholes and the rest of the fracture plane.

For the radially converging test only one realisation of the head field was made. However, several simulations of the tracer tests were made using different positions for the injection holes. The position were selected so that they in each simulation were at the same distance from the pumping hole and did not deviate more than 10 degrees from the actual direction. The latter requirement is due to the regional head gradient used.

The fixed hydraulic head values set on the boundaries were calculated by fitting a linear model to the calculated natural fresh water heads before the start of the radially converging tracer test and extrapolating the head values to the boundary.

The alternative model was used to simulate the transport between KXTT1 to KXTT3 assuming transport in a single 5 cm wide channel. The transport velocity was calibrated based on the results of the preliminary tracer test.

Dipole tests

The transmissivity field used in the radially converging test was also applied to the dipole tests. However, in this case the part of the fracture closer than 0.3 metres to all boreholes were assigned a higher transmissivity value ($3\cdot10^{-5}$ m^2/s) to ensure a sufficient hydraulic conductivity between the boreholes and the rest of the fracture plane. A set of 30 different realisations of the head field was generated and predictions for all four dipoles were made for each realisation.

When using a regional gradient by fitting a linear model to the measured hydraulic head values it appeared that no recovery from any of the dipole tests was possible with the selected transmissivity field. The measured head field has significantly changed over time and was therefore regarded as uncertain. Thus, a fixed zero head boundary was used for the predictions of the breakthrough.

The alternative model was applied only to the DP-1 test. Seven flow channels were simulated each 5 cm wide. The channel lengths, flow rates and transport velocities were derived from a two-dimensional homogeneous flow model. The ratio between the transport aperture and the hydraulic aperture was assumed to be 10.

3.2.6 BMBF/BGR

The Federal Institute of Geosciences and Natural Resources (BGR) supported by the Federal Ministry of Education, Sciences, Research and Technology (BMBF) of Germany has participated in the Task 4C/4D modelling work with the purpose of improving knowledge of flow and transport mechanisms in fractured rock and testing methods of studying them. An additional purpose of participating is the possibility to exchange experience with international partners, e.g. from the in-situ experiments performed at the Grimsel site in Switzerland where BMBF/BGR has participated. The BMBF/BGR group specially wants to address the influence of flow heterogeneity of fracture systems on the flow system and the understanding of solute transport in the geosphere interpreted from a detail scaled in-situ experiment.

The features within the TRUE-1 block have been treated as two-dimensional planar structures (Liedtke and Shao, 1997). In the initial modelling both Feature A and B were included in the model. However, the hydraulic influence of Feature B on Feature A was found to be negligible, due to the large difference in transmissivity. Thus, only Feature A was given attention in the subsequent modelling. The feature was modelled using a uniform grid with dimensions 20 x 20 m with hydraulic properties given by hydraulic conductivity and fracture aperture. The flow in the feature was obtained by solving the flow equation. Both cases with homogeneous and heterogeneous hydraulic properties were studied. In the heterogeneous models, 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 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 tracer transport was simulated with the advection-dispersion equation using the calculated water velocity field from the flow model. Hydrodynamic dispersion and molecular diffusion are described as a Fickian process. Diffusion into the rock matrix was not included. The injection of tracer was modelled using a time dependent concentration at boundary representing the injection segments corresponding to the experimental concentrations. This caused, in some cases, a total injected mass different from that of the experiment, since the total injected mass in the experiment was unknown, and the flow rate through the injection section could differ considerably between the model and the experiment. In order to compensate for this, a correction factor was introduced based on the actually injected amounts of tracer.

Radially converging test

A predictive calculation of the radially converging test was made using a deterministic homogeneous model of Feature A with values of the flow and transport parameters determined by calibration of the model on the results of the preliminary tracer test. The hydraulic conductivity and equivalent fracture aperture were close to those presented by Winberg (1996). In the transport calculations also an effective porosity within the fracture of 0.4 was included. A longitudinal dispersion length of 0.4 m and transversal dispersion length of 0.12 m were used. Corrections of the amount of injected tracer were made.

Dipole test

The hydraulic conductivities and fracture apertures were adjusted based on the results of the radially converging test. Two different meshes were used. In the first mesh, the only adjustment was a local decrease in hydraulic conductivity and an increase in aperture around borehole KXTT3, based on the pressure differences between the injection holes and the pumping holes and the tracer breakthrough time. In the second mesh, the constant fracture aperture was kept, but the hydraulic conductivity in areas around the boreholes was calibrated to fit the measured drawdown. Artificial dipole flow fields were superimposed on the natural head distribution prior to the dipole tests. The transport calculations were made using the same parameters as in the radially converging test.

3.2.7 SKB/KTH-TRUE

The modelling team from Royal Institute of Technology/Water Resources Engineering of Sweden and SKB is part of the TRUE Project team. The predictions for Tasks 4C/4D are a part of the predictions/evaluations made within the TRUE programme, following the overall objectives given by the TRUE programme. The team has focussed their modelling work on studying the effect of a heterogeneous transmissivity distribution within Feature A (Selroos and Cvetkovic, 1998). The SKB/TRUE team especially wants to address the possibility to increase the understanding of flow and transport and decrease the uncertainty in predictions by using conditioning of the stochastic fields on available data. The possibility of comparison with results from flow and transport experiments is therefore essential. The modelling has an emphasis on the flow description, i.e. transmissivity and head data, while the transport modelling is largely determined by calibration to the measured breakthrough in the preliminary tests.

The feature is modelled as a single two-dimensional plane with dimensions 20 by 20 metres. The effect of connecting fractures was assumed to be small based on the hydraulic-structural investigations performed. However, the effect of the tunnel is acknowledged to be of importance for the gradient and thereby also for the transport. The assumption of a singular fracture is judged to be most significant and can, if proven wrong, lead to misleading conclusions.

The flow in the feature is described by the two-dimensional flow equation using a spatially variable transmissivity with an assumed distribution and correlation length (stochastic continuum approach). In some of the calculations also the effect of a homogeneous transmissivity has been studied. The calculations were performed on an equidistant mesh with an element size of 0.4 meters. The thickness of the feature is assigned a constant value corresponding to an effective aperture. The transport in the feature is described by a Lagrangian travel time approach where individual numerical particles are tracked in the velocity field. The number of particles was 100. In the present case diffusion or local dispersion have not been considered, i.e. dispersion is only caused by the spatially variable flow velocity. The travel times along the streamlines are solved for a pulse injection and the effect of the actual source term is accomplished by superpositioning solutions for different time of injection.

Radially converging test

Multiple realisations of unconditional and conditional transmissivities have been generated using the Monte Carlo approach. Two types of conditioning were made, in the first case based on measured transmissivities in the boreholes and steady-state heads in the boreholes prior to pumping, and in the second case based on transmissivities, head values prior to pumping and head values during steady-state pumping in one interference test.

The boundary condition for the unconditional case was a uniform head set to all boundaries, with a head value taken from KXTT3. For the conditional cases the boundary conditions were obtained by extending approximate head isolines from the boreholes (no pumping) out to the boundaries, assuming that the boundaries are unaffected by the subsequent pumping during the test. This resulted in a regional gradient from KXTT4 towards KXTT3.

For the predictions of the radially converging tracer test, transmissivity measurements from the interference and pressure build up tests have been used as a basis for the assumed spatial lognormal distribution of the transmissivity. This gave a mean m_Y=-7.5 and a variance of $\sigma^2_Y = 0.4$, where $Y=\log_{10}(T)$. A correlation length of 1 metre was assumed. However, the conditioning procedure changes the transmissivity such that the statistics of the realisations by increasing the mean transmissivity and the variance compared to the input statistics. The constant effective aperture was in each of the predictions calibrated to give a median breakthrough time for recovery of half the mass, T_{50}(50%), consistent with the mean travel time from the preliminary tracer test. Thus, the flow conditioning is of a more generic nature while the transport calibration serves more as a fitting parameter.

Dipole tests

The boundary conditions were revised for the prediction of the dipole tests. In this case approximate unstressed isolines based on the head values in the boreholes prevailing prior to the start of the radial converging test were extended out to the boundaries. The new boundary conditions resulted in a regional gradient from KXTT3 down towards KA3005. Furthermore, simulations both with a homogeneous transmissivity and cases with heterogeneous transmissivity fields were made. The transmissivity fields are conditioned on measured transmissivities and steady-state head values prior to and during pumping of KXTT3 in the radially converging experiment. These head values from the RC-1 test were judged to be more relevant than those obtained during the interference test, since the used flow rate was much closer to the ones used in the dipole experiments. A spatial distribution with a mean m_Y=-7.7 (interference test only), a variance of $\sigma^2_Y = 0.4$ and a correlation length of 1 metre was used as a starting point for the conditioning.

The effective aperture was in this case calibrated against the mean travel time for the flow path between KXTT1 and KXTT3 in the radially converging experiment.

The dipole tests provided a good opportunity to test the conditioning capability since several different pumping combinations were available. In RC-1 the conditioning as well as all prediction was performed on pumping in KXTT3, while in the dipole tests conditioning was performed on pumping in KXTT3, but the predictions were for pumping in three different boreholes.

Sensitivity analysis has been performed on the sets of transmissivity fields generated for the radially converging and dipole experiments. The following variants are studied: a correlation length of 0.5 metres, an uncertain boundary condition on the domain boundary, a combination of these two variants and a variant with a finer discretisation (element size 0.2 metres).

3.2.8 ANDRA/CEA-DMT

The Agence Nationale pour la Gestion des Déchets Radioactifs / Commissariat a l'Energie Atomique Direction des Reacteurs Nucleaires-Departement de Mécanique et de Technologie (ANDRA/CEA-DMT) has participated in the Task 4 modelling work presenting predictive results for the radially converging test (Mouche et al., 1996).

The ANDRA/CEA-DMT team has modelled the feature A as a two-dimensional infinite fracture using a stochastic approach. The mean flow is assumed to be radial and calculated using the equation for radial flow neglecting the natural gradient. The transmissivity field was assumed to be weakly heterogeneous with a lognormal distribution. In the transport calculations, the dispersion is taken in account but not the molecular diffusion. The dispersivity values were deduced from the preliminary tracer tests.

The flow equations were solved analytically, but the transport equations were solved with a numerical model based on the mixed hybrid finite element code CASTEM2000. A sensitivity analysis has been performed including variation of mesh size, time step, borehole distances and dispersivity values. The calculation of the mean and the standard deviation of the concentration in the pumping borehole was made by convolution of the injected concentration with the time derivative of the concentration due to a unit injection of a concentration step. The framework of the mesh is quadrangular and the number of elements varies between 50 and 200 depending on the experimental configuration.

Radially converging test

In the predictive calculations of the radially converging test the calculations were made for the assumptions of radial flow and purely radial transport. The mean transmissivity was taken from Winberg (1996) and the equivalent fracture aperture assumed to be 1 mm. The statistics for the transmissivity were unknown during the modelling, therefore a standard value based on values from the literature was used in the calculation of flow. The boundary conditions used were: at the pumping borehole a dispersive flux equal to zero, and at the injection borehole the injection concentrations. The dispersivity determined from the preliminary test was used. Also calculations were made for value half of the original, in order to study the sensitivity of the results.

3.2.9 AEA Technology

The AEA Technology team has participated in the Task 4 modelling work presenting predictive results for the radially converging test. One purpose of the modelling has been to evaluate the consequences of a simple variable aperture conceptual model for an isolated fracture.

The AEA Technology team has modelled the Feature A as a two-dimensional heterogeneous fracture with the dimensions 25 x 20 meters (Worraker et al, 1998). The distribution of the fracture aperture has been modelled as a stochastic process and the stochastic properties have been based on measured or interpreted values of transmissivity and hydraulic head. It is noted that if the transmissivity (T) is log-normally distributed then so is the aperture (e) based on the linearity of the relationship between log(T) and log(e). The transmissivity fields were conditioned on the known values of the transmissivity using kriging. The flow field in the fracture was solved using Darcy's law assuming that the local transmissivity is a function of the cube of the local fracture aperture. For each studied case 100 stochastic realisations of the flow field were made. The advective component of the flow was determined by calculating pathlines in the flow field. For each pathline, the transport was calculated by solving the advection-dispersion equation on the resulting one-dimensional stream tubes. Dispersion was assumed to be due to velocity differences across the fracture (Taylor dispersion). The flow calculations and the transport calculations were solved with a numerical model based on the finite element code NAMMU. The number of elements in different simulations varied between about 2000 and 4300, with the results showing grid convergence. The mesh was refined in the central part where the boreholes were located.

Radially converging tests

Four variants were considered to calibrate the model against the preliminary tracer test. The data for the last variant was used to make predictions for the radial converging test. In the initial calculations the transmissivity was assumed to have a lognormal distribution with parameters based on the single packer flow logging (Winberg, 1996). However, the values were in the last variant adjusted to simulate the drawdown in the preliminary tracer test. In the flow calculations different boundary conditions were analysed. In the first variants a fixed head was kept on two boundaries, while the other two were considered no flow boundaries. In the later variants, the boundary conditions were modified to more closely match the unperturbed head field. In the transport calculations the dilution source was modelled using a convolution procedure with decay constant. The decay constants were calculated by linear fitting of the later time data from the dilution curves in the injection boreholes from the preliminary tracer test.

4 Results

4.1 Modelling results

This section gives a brief overview of the modelling results. A more comprehensive compilation of results is given in Ström (1996 and 1997) and in the ICR reports written by the modelling groups.

One of the major differences between the presentation of the results is that some of the modelling groups have used deterministic models and others have used stochastic models, consequently some results are given with percentile intervals and some as point estimates. Table 4-1 shows the modelling approach the different groups have used.

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

Modelling group	Stochastic	Deterministic
CRIEPI	X	X
PNC/Golder	X	X
SKB/KTH-ChE	X	
Posiva/VTT	X	X
BMBF/BGR		X
SKB/KTH TRUE	X	X
ANDRA-CEA	X	
Nirex/AEA	X	

All modelling groups have presented their results according to the instructions from the SKB Task Force Secretariat, i.e. steady state drawdown in the pumping and injection sections, 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.

Figure 4-1 shows an example of the results from the RC-tests with deterministic results (BMBF/BGR and PNC/Golder) and the result of two stochastic models (CRIEPI and SKB/KTH-TRUE).

In Figure 4-2 the predictive breakthrough curves for dipole test DP-1 are shown. The results of the teams who have used a stochastic approach are presented by the 50-percentile.

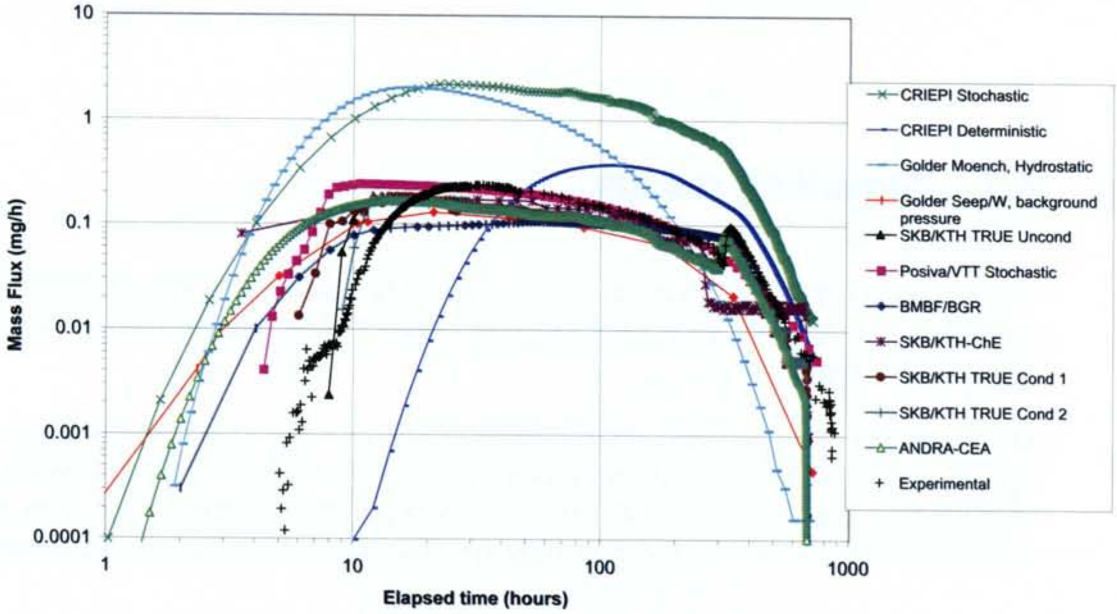

Figure 4-1 Breakthrough curve from test between KXTT1 R2 and KXTT3 R2 in the RC-1 test.

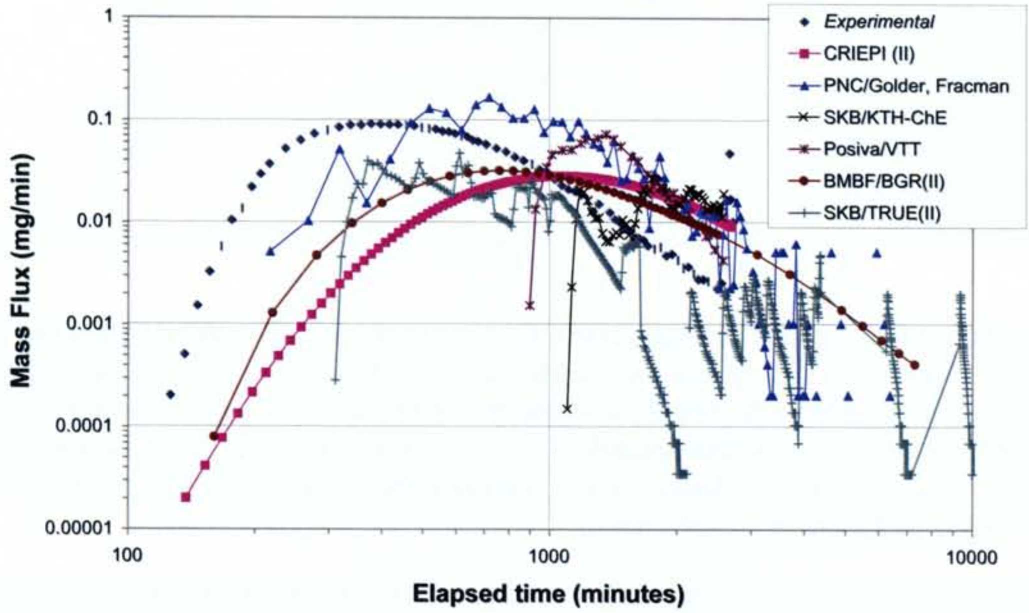

Figure 4-2 Breakthrough curve from dipole test between KXTT1 R2 and KXTT3 R2 in the DP-1 test.

4.2 Experimental results

4.2.1 Radially converging tracer test (RC-1)

In the borehole sections KXTT1 R2, KXTT2 R2, KXTT4 R3 and KA3005 R3 two tracers were injected in each section, a fluorescent dye and a metal complex. With pumping in KXTT3 a radially converging flow geometry was achieved. While pumping, the tracer breakthrough from all four injection sections was monitored in KXTT3. However, after more than two weeks no breakthrough was detected from the boreholes furthest away, i.e. KXTT2 and KA3005. An increase in the pumping rate was therefore made from 0.2 l/min to 0.4 l/min, and later further increased to 3 l/min. With increased pumping rate tracers from these boreholes could be detected in the pumping hole. Figure 4-3 shows the injection curve for KXTT1 R2 and the obtained breakthrough in KXTT3 R2. The sharp increase in both tracer injection and breakthrough observed after about 320 hours, see Figure 4-3, is due to the permanent flow increase through the injection section in KXTT1 caused by the releasing of gas from the injection section in borehole KXTT2 prior to the tracer injection there. The breakthrough curve from the injection in KXTT4 is presented in Figure 4-4. In both cases the injection curves and the breakthrough curves have a similar shape due to the long residence time in the injection section compared to the travel time in the feature. The experimental error in the mass flux was estimated to be in the order of 2%.

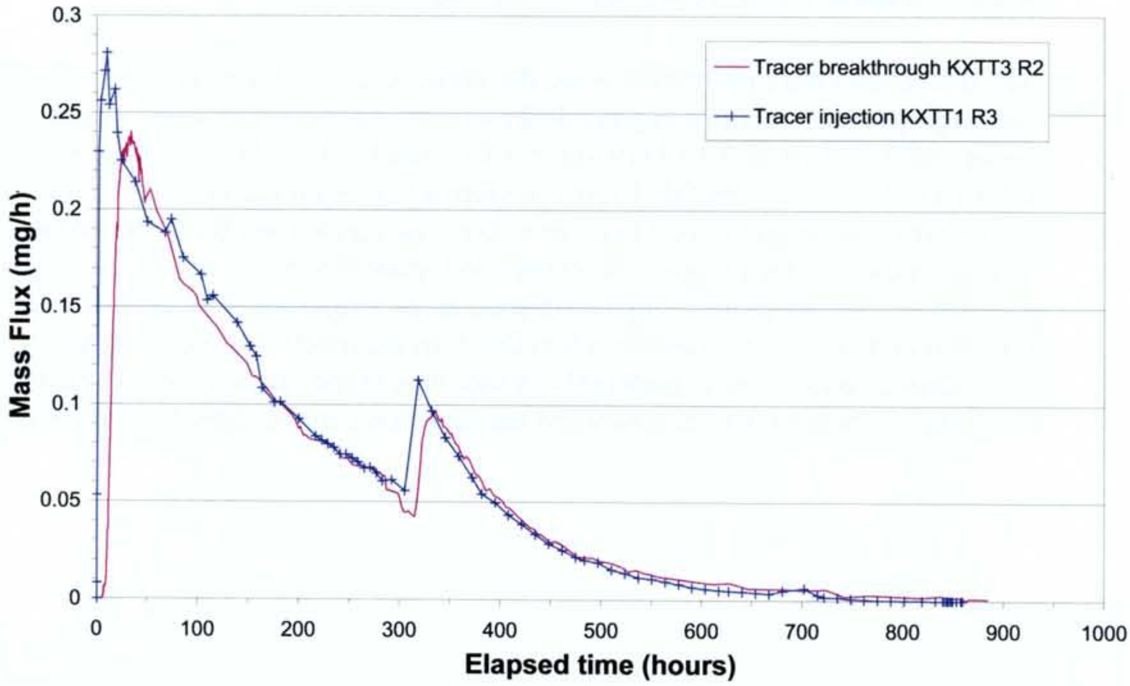

Figure 4-3 Comparison between output and input mass flux for the test between KXTT1 R2 and KXTT3 R2 in the RC-1 tests.

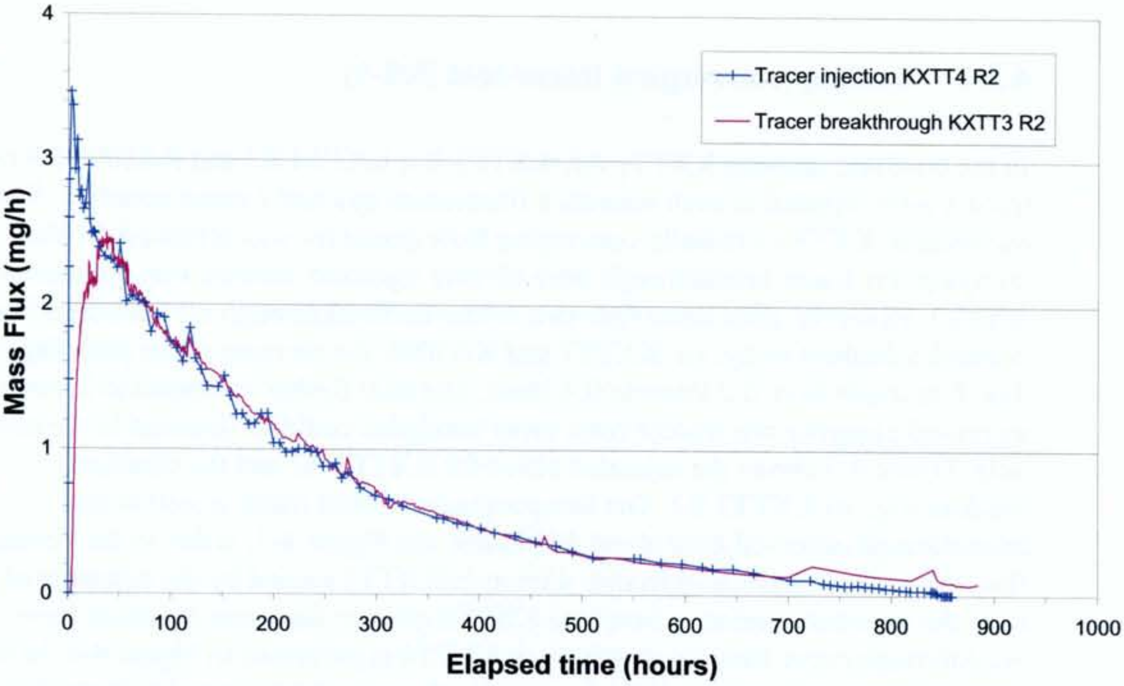

Figure 4-4 Comparison between output and input mass flux for the test between KXTT4 R3 and KXTT3 R2 in the RC-1 test.

4.2.2 Dipole tracer tests (DP 1 – DP 4)

The dipole tests were performed using the same extraction holes as in the radially converging tests, but with a slightly different configuration. The dipoles were set up between KXTT1 and KXTT3 (DP-1), KXTT2 and KXTT1 (DP-2, DP-3), KXTT2 and KXTT4 (DP-4). Thus, the DP-1 test is performed between the same boreholes as one of the radially converging tests. Fluorescent dye was injected and the breakthrough curves were monitored in the pumping boreholes. In Figure 4-5 the breakthrough curves of the four dipole tests are plotted. Figure 4-6 presents a comparison between the tracer injection and the tracer breakthrough in DP-1. In the dipole test the residence time in the injection section was considerably shorter than in the radially converging test, resulting in a better separation between the injection curve and the breakthrough curve.

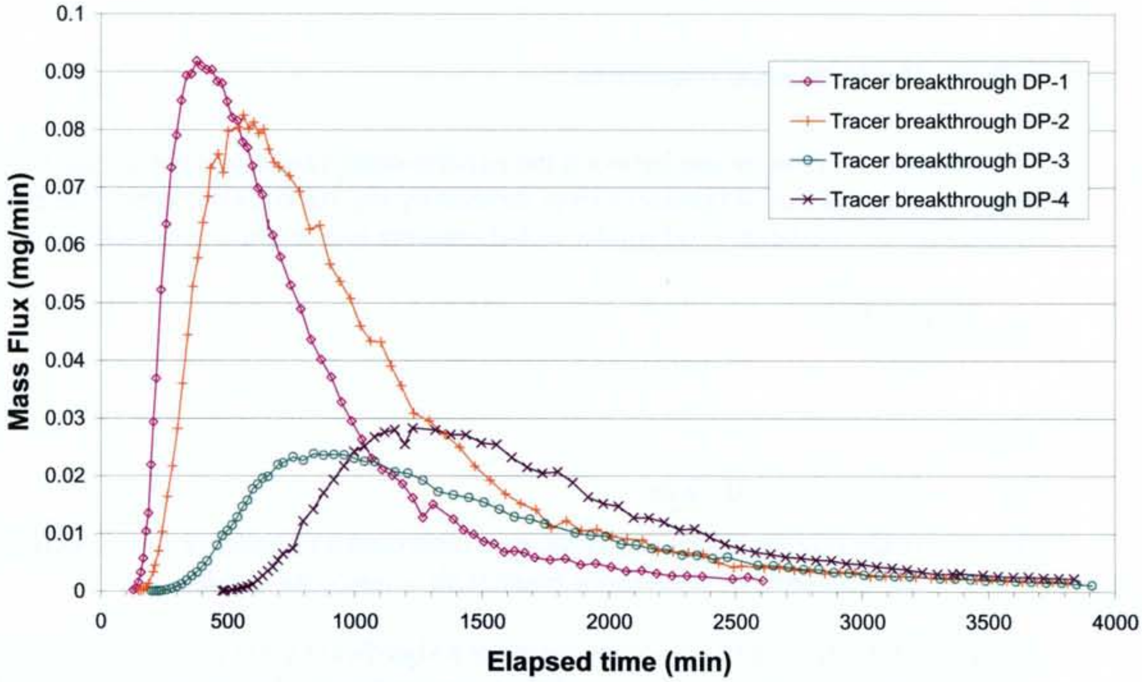

Figure 4-5 Comparison between measured breakthrough curves in the dipole tests DP-1 – DP-4.

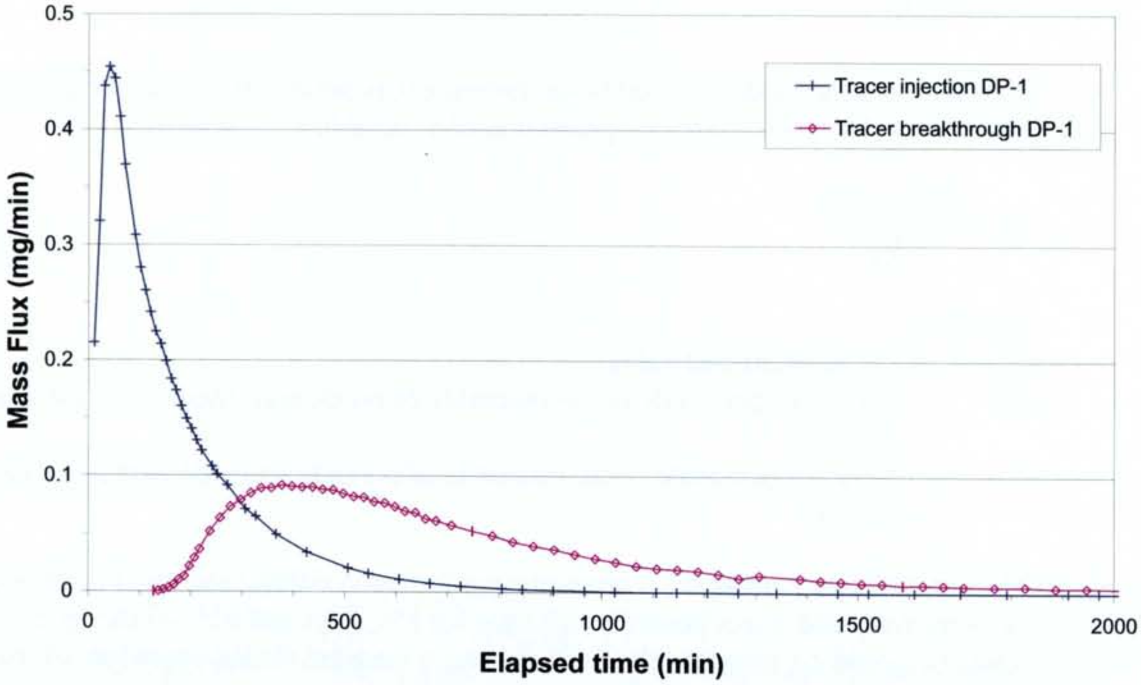

Figure 4-6 Comparison between output and input mass flux for the flow in the DP-1 test.

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:

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

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. An alternative would be to use the logarithm of the ratio between the predicted and the measured value:

$$A = \log \frac{X_m}{X_p} \qquad (4\text{-}2)$$

For the stochastic models an additional measure was defined for the uncertainty in the predictions. The uncertainty in a prediction of a variable X is given by:

$$U = \frac{(X_{95} - X_5)}{X_m} \qquad (4\text{-}3)$$

where:

X_m is the measured value.

X_{95} is the 95-percentile of the ensemble of predictions made with a stochastic model

X_5 is the 5-percentile of the ensemble of predictions made with a stochastic model

These performance measures were evaluated for the variables: steady-state drawdown, mass recovery and tracer breakthrough time for 5%, 50% and 95% of the recovered mass, t_5, t_{50} and t_{95}, respectively. Furthermore, a measure for the spreading of the breakthrough in time, D_t, was defined as: $D_t = t_{95} - t_5$.

4.3.2 Radially converging test

Drawdown

In general the models overpredicted the drawdown in all of the observation wells. The differences were in many cases quite large, see Table 4-2. The exceptions were the SKB/KTH-TRUE unconditioned model which gave predictions with an error in the prediction (accuracy) as defined by Equation 4-1 between -1.69 and 0.76, and the PNC/Golder FracMan model which underpredicted the drawdown.

Table 4-2 Predicted and observed drawdown (meters) in the radially converging test. Median values used for the stochastic models.

MODELS	KXTT1	KXTT2	KXTT4	KA3005A	KXTT3
CRIEPI Stochastic	15.3	12.6	17.1	8.7	60.6
CRIEPI Deterministic	4.6	3.79	7.47	2.87	128.3
PNC/Golder Moench, Hydrostatic	2.59	2.25	2.68	1.79	8.22
PNC/Golder SEEP/W Local press.	5.02	0	5.34	0	-
PNC/Golder Fracman Hydrostatic	0.5	0.6	0.9	0.4	1.7
PNC/Golder SEEP/W Hydrostatic	6.03	6.32	5.96	6.7	-
SKB/KTH-ChE	3.22	2.8	3.68	2.03	12.22
POSIVA/VTT	2.29	0.57	2.01	0.43	7.18
BMBF/BGR	3.54	2.53	2.95	1.61	9.0
SKB/KTH True Uncond	0.75	0.53	0.86	0.28	4.2
SKB/KTH True Cond 1	4.98	3.89	3.87	2.71	77.82
SKB/KTH True Cond 2	4.62	9.42	1.43	2.55	12.61
Nirex/AEA	0.94	0.71	0.10	0.39	6.50
Experimental	***0.62***	***2.23***	***0.32***	***0.28***	***3.12***

Mass Recovery

During the experimental time an almost complete recovery was obtained from two of the injection holes, KXTT1 and KXTT4, (91% and 97% respectively), while no tracer was recovered from the injections in KXTT2 and KA3005A. As shown in Table 4-3 only a few of the models predicted the absence of recovery from the KXTT2 and KA3005A. The Posiva/VTT and CRIEPI models predicted a significantly lower recovery from injection in these holes and the PNC/Golder based on the local head and regional head boundary conditions predicted low or no recovery from KXTT2 and KA3005A.

Table 4-3 Predicted and observed mass recovery (%) in the radially converging test. Median values used for the stochastic models.

MODELS	KXTT1	KXTT2	KXTT4	KA3005A
CRIEPI Stochastic	100	90	100	83
CRIEPI Deterministic	99.3	52.3	99.8	63.1
PNC/Golder Moench, Hydrostatic	100	99	82	78
PNC/Golder SEEP/W, Local head	100	0	100	0
PNC/Golder Fracman, Hydrostatic	99	100	100	45
PNC/Golder SEEP/W, Hydrostatic	100	100	100	100
PNC/Golder Moench, Regional Head	50	5	5	0
PNC/Golder Moench, Dilution Head	100	99	82	40
PNC/Golder Moench, Local Head	100	0	100	0
PNC/Golder SEEP/W, Regional Head	6.5	0	12.5	0
PNC/Golder Fracman, Regional Head	90	20	60	5
SKB/KTH-ChE	100	99	100	65
POSIVA/VTT	98	31	96	26
BGR	157.6[1]	100.2	135.4[1]	101.1
SKB/KTH True Uncond	100	100	100	92
SKB/KTH True Cond 1	100	100	100	95
SKB/KTH True Cond 2	100	100	100	92
Experimental	***91***	***0***	***97***	***0***

Notes: [1] Due to overestimation of the flow rate in the injection sections of KXTT1 and KA3005A a mass recovery exceeding 100% was obtained.

Breakthrough

The models generally underpredicted the first breakthrough time for the tracers injected in KXTT1 and KXTT4, while the prediction of the median breakthrough time generally was quite good, see Figure 4-7. The predictions of the injection in KXTT4 had in general an equal or better accuracy than for the injection in KXTT1, despite the fact that most models were calibrated on the preliminary tracer test performed between KXTT1 and KXTT3.

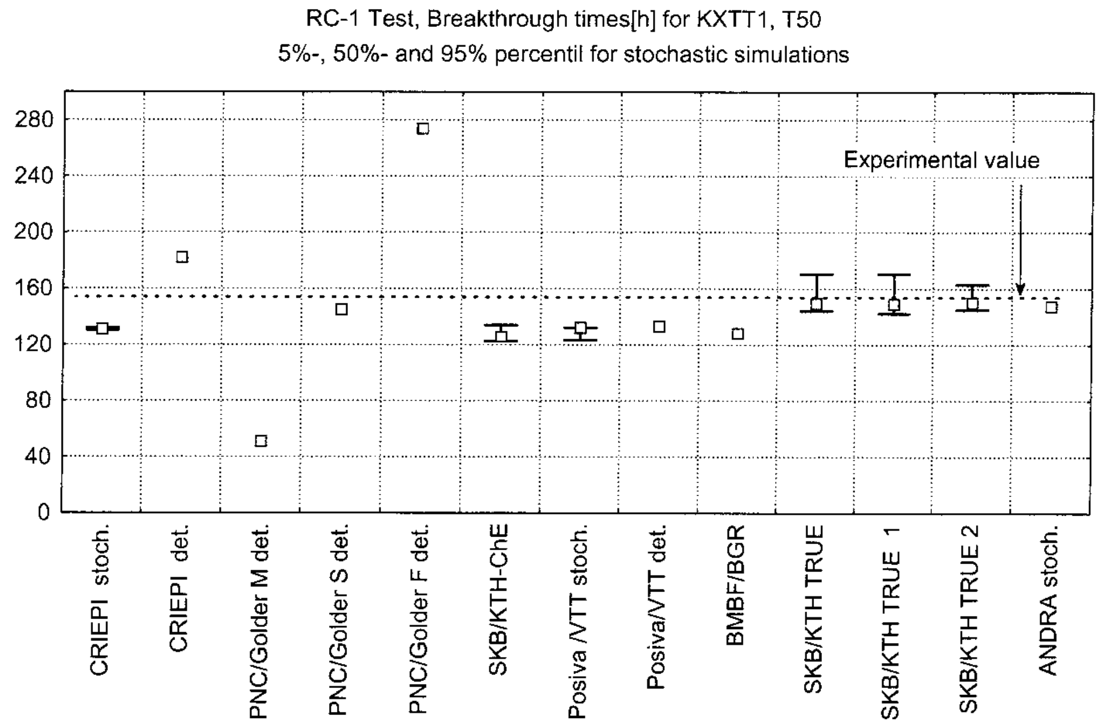

Figure 4-7 Predictions of median breakthrough time (in hours) for injection in KXTT1 (5, 50 and 95-percentiles for stochastic models).

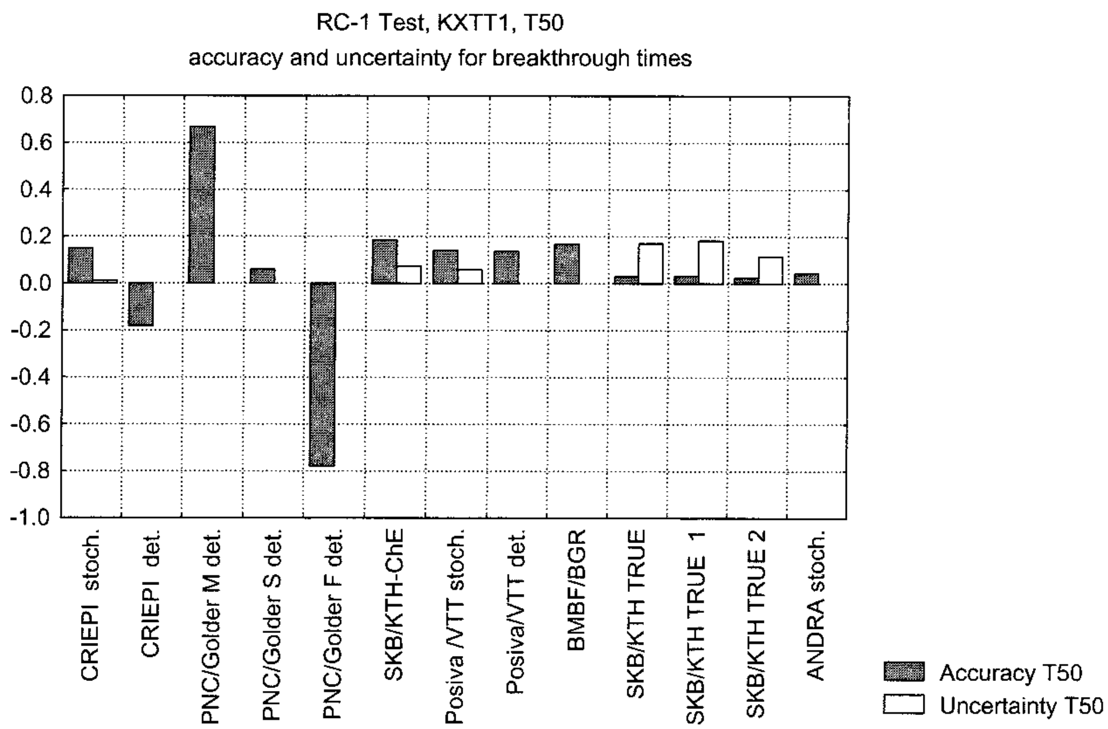

Figure 4-8 Performance measures for predictions of median breakthrough time for injection in KXTT1 with accuracy as originally defined (Eq. 4-1).

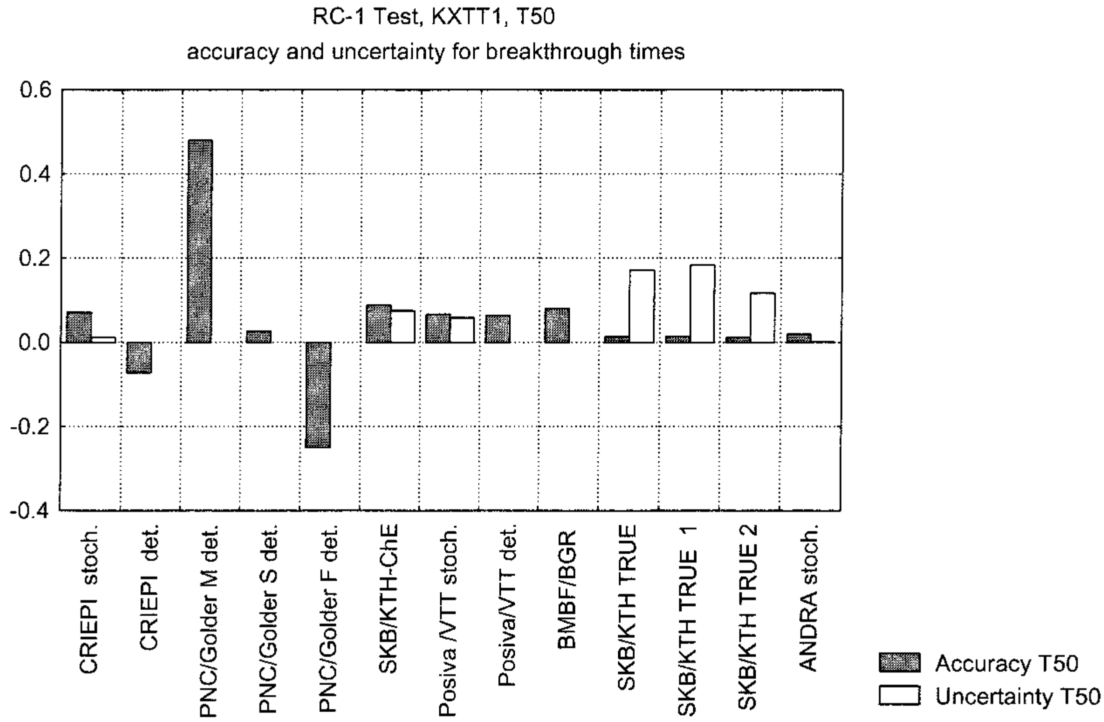

Figure 4-9 Performance measures for predictions of median breakthrough time for injection in KXTT1 with alternative definition of accuracy (Eq. 4-2).

4.3.3 Dipole tests

Drawdown

The prediction of the drawdown in KXTT3 during the DP-1 test was quite accurate for all modelling groups, see Figures 4-10 and 4-11. For this dipole test accurate predictions could also be expected, due to the calibration and conditioning made on the results of the radially converging test. However, all models except the SKB/KTH-TRUE stochastic model considerably underestimated the drawdown due to the pumping in KXTT1 in DP-2 and DP-3. Also the drawdown due to pumping of KXTT4 during DP-4 was greatly underestimated except by the SKB/KTH-TRUE stochastic model and the BMBF/BGR Mesh 2 model. However, the uncertainty in the SKB/KTH-TRUE stochastic model results was quite large. Also the head increase due to the injection in dipoles was greatly underestimated by all models.

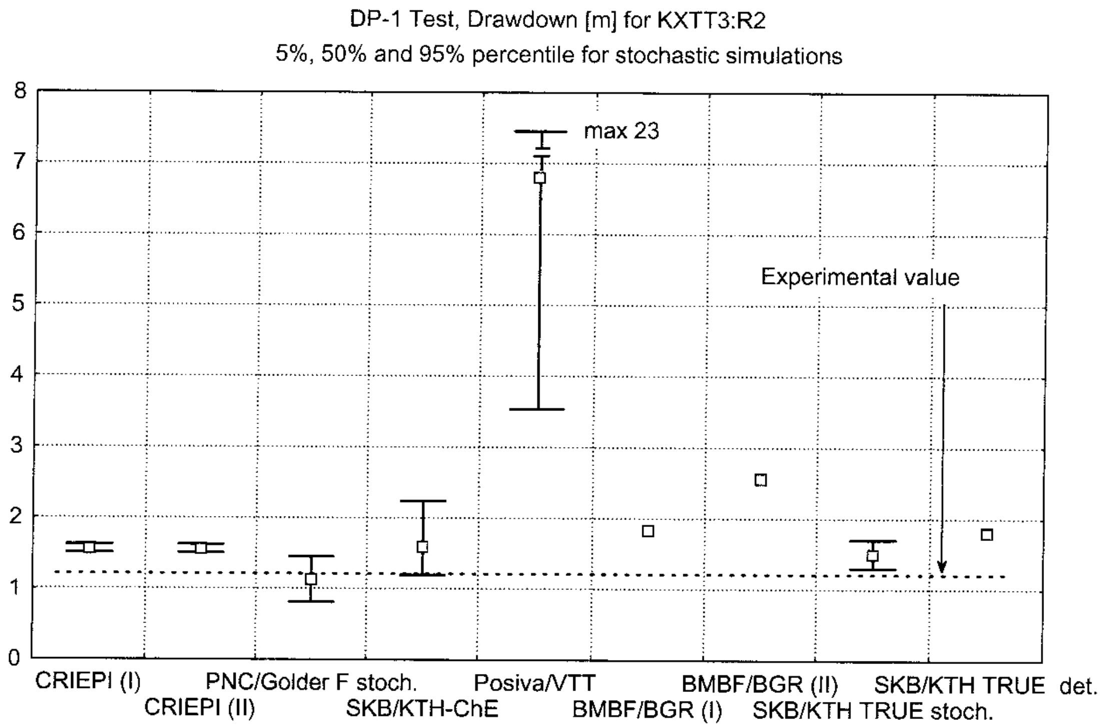

Figure 4-10 Predictions of drawdown (in metres) in KXTT3 during DP-1. (5, 50 and 95-percentiles for the stochastic models.)

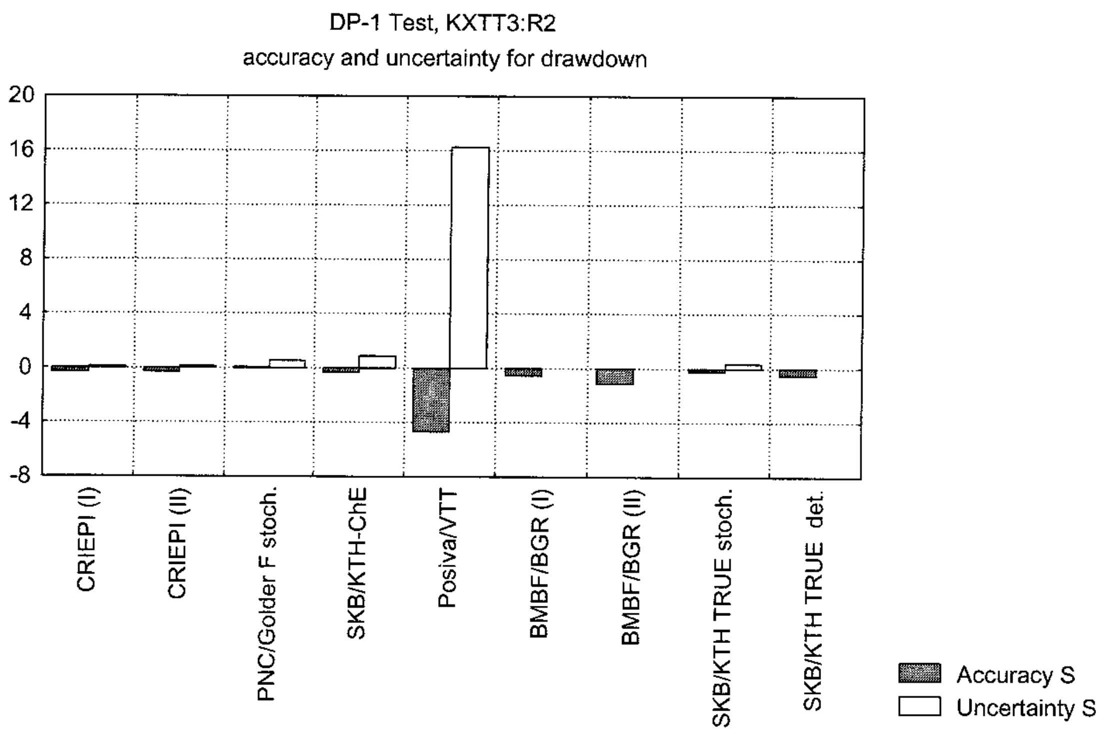

Figure 4-11 Performance measures for predictions of drawdown in KXTT3 during DP-1. (5, 50 and 95-percentiles for the stochastic models.)

Mass recovery

All models, except Posiva/VTT underestimated the mass recovery in DP-1. However, the uncertainty ranges were for several of the stochastic models quite large, with the experimental value within the range. Most models predicted the limited recovery that was observed in DP-2, DP-3 and DP-4. However, there was a large spread in the prediction and in several cases very low mass recovery was predicted.

Breakthrough

The breakthrough time (t_5 and t_{50}) for DP-1 was generally overpredicted by a factor of 1.5 to 3.6, see Figure 4-12. The median value of the SKB/KTH-TRUE stochastic model was close to the experimental. For this model no 95-percentile was calculated since due to numerical problems more than 5% of the simulations resulted in no recovery. The overprediction of the median breakthrough time is inconsistent with the accurate predictions of the same configuration in the radially converging test and somewhat surprising considering that more information should be available concerning the flow path between KXTT1 and KXTT3. The predictions of the median breakthrough time made for the other dipoles give values both lower and higher than the experimental. However, the predictions for the other dipoles are in most cases more accurate than for DP-1.

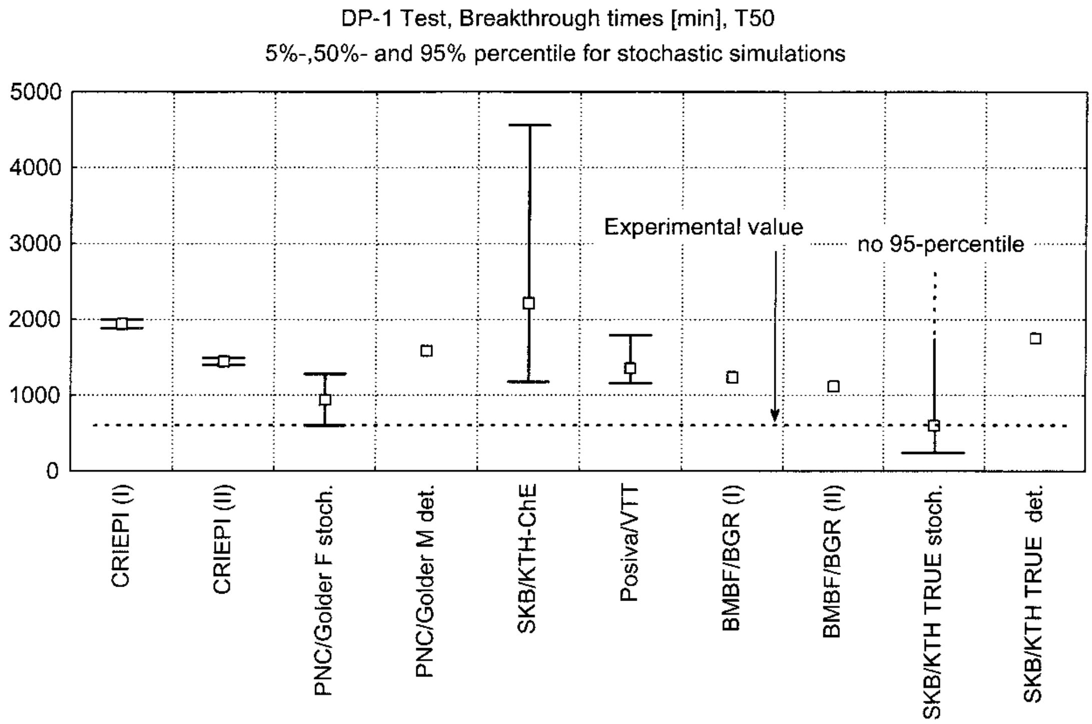

Figure 4-12 Predictions of median breakthrough time (in hours) for DP-1. (5, 50 and 95-percentiles for the stochastic models.)

5 Discussion

The disposition of this chapter is based on that of the questionnaire concerning Tasks 4C and 4D. The discussion focuses on issues brought up by the modelling teams in their response to the questionnaire and in their modelling reports. A compilation of the questionnaire responses from the different modelling teams is given as Appendix 3.

5.1 Model geometry and structural model

All of the modelling teams have based their computational model on the available structural-hydraulic model of the TRUE-1 site (Winberg, 1996). The PNC/Golder group has in addition used information from the discrete fracture analysis in support of TRUE-1 (Dershowitz et al., 1996). The majority of modelling groups considered Feature A as an isolated single feature, which could be motivated by the relatively limited connectivity to other features found in the site characterisation investigations. The large pressure difference found between the Features A and B indicates a weak connectivity between the features. The BMBF/BGR group also included Feature B, but found in their preliminary calculations that it had negligible hydraulic influence on Feature A in the experimental configurations used.

Another reason for limiting the model to a single feature is the relatively large number of local head measurements available in Feature A (Dershowitz et al., 1998). For this reason the PNC/Golder team chose to consider their discrete fracture network model as a supplementary model in the predictive modelling. A large scale DFN-model could not be expected to give a better representation of the local head field than what was available from the measurements. However, such a model could be useful in interpreting and understanding the global impact on the head field in Feature A.

The SKB/KTH-ChE is the only group that has explicitly included the tunnel in the modelling, although other groups (e.g. SKB/KTH-TRUE) acknowledge its potential importance. However, the inclusion of the tunnel is not straightforward due to the changes in hydraulic properties caused by the excavation. The SKB/KTH-ChE group chose to describe this by decreasing the conductivity of any channels connecting with the tunnel by a given factor.

5.2 Modelling of processes

All modelling groups have included a similar set of processes. For a summary of processes, see Table 3-1. The water flow is modelled as Darcy flow determined by head gradients and transmissivity/hydraulic conductivity. The main difference is in the degree of detail by which the flow paths within the features are described, see Section 5.3.

A number of modelling teams has specifically stated that heterogeneous flow is an issue they want to address in Task 4. This has either been done by stochastic continuum modelling, where flow paths are generated by high transmissivity parts of the domain (CRIEPI, Posiva/VTT and SKB/KTH-TRUE) or by explicitly modelling the flow paths as channels (SKB/KTH-ChE). The BMBF/BGR team has chosen to deterministically assign different properties to the modelled features and thereby study the effect on flow and transport. However, the PNC/Golder team has chosen to treat Feature A as homogeneous and to a large extent focussed on other issues, e.g. boundary conditions and connecting fractures. The reason for not using a stochastic continuum model was that the preliminary tracer experiment indicated little dispersion. The PNC/Golder team considered the presence of multiple flow paths with different properties not probable and therefore concluded that a stochastic continuum model generating a varying transmissivity field would likely overestimate dispersion within Feature A. However, in their discrete fracture network model a highly conductive feature was included in between boreholes KXTT2 and KXTT3 to be able to describe the large drawdown in KXTT2.

All modelling groups have considered advection as the main transport process with dispersion as a secondary process, see Table 3-2. There are considerable differences concerning to what extent dispersion is included and in the way by which it is described. The SKB/KTH-ChE, and SKB/KTH-TRUE teams have only considered the hydrodynamic dispersion due to the presence of several flow paths with different residence times. The same applies for the main model of the Posiva/VTT team, with the addition that molecular diffusion is considered as a random component in the particle tracking. However, in the present situation molecular diffusion in the fracture is of little importance. The CRIEPI, PNC/Golder and BMBF/BGR modelling teams have described hydrodynamic dispersion using a dispersion coefficient either using the advection-dispersion equation or as a random component in the particle tracking.

In the performed tracer experiments matrix diffusion is of little importance due to the short travel times and the use of conservative tracers. The only model including matrix diffusion is the SKB/KTH-ChE model.

5.3 Material properties

The hydrological properties assigned to Feature A are based on the results of the performed site characterisation. In general, the starting point has been the transmissivity values given in the site characterisation report (Winberg, 1996). In this report the transmissivities of the borehole sections were determined from three different tests (pressure build-up tests, single packer flow logging, and interference tests). Furthermore, an analysis of fracture conductivity and mass balance aperture from the preliminary tracer test can be used to determine the fracture transmissivity. The modelling teams have in many cases adjusted the data from Winberg (1996) in order to obtain a better fit of their models to the performed experiments. In Table 5-1 a summary is given of the flow and transport parameters used by the different modelling teams.

Table 5-1 Summary of used parameters (values for lognormal distributions given in base 10)

TOPIC	CRIEPI	PNC/Golder(I)	PNC/Golder(II)	PNC/Golder (III)	SKB KTH-ChE	POSIVA/VTT	BMBF/BGR	SKB KTH-TRUE	Nirex/AEA	Andra
Type of model	Deterministic continuum model (Stochastic in predictive modeling)	Analytical model	Deterministic continuum model	Discrete fracture network model (DFN)	Channel network model	Stochastic continuum model	Deterministic continuum model	Stochastic continuum model	Stochastic continuum model	Analytical model/linear stochastic model
Hydraulic head	All surrounding boundaries: fixed hydraulic heads.	Hydrostatic head (360 m) at infinite distance	1) Hydrostatic head (360 m) on the model edges. 2) Head on edges consistent with head in boreholes.	Hydrostatic head (360 m) on the model edges.	Head on model edges -40 m. Head at tunnel -392 m.	RC: Head on edges extrapolated from measurements in boreholes. DP: Fixed zero head on boundaries.	Fixed hydraulic head (-41m) at top of feature A and at a point on north side (-42) to simulate natural flow conditions.	Head boundary conditions on all boundaries, extrapolated from boreholes.	Variant A: 4E5 Pa on sides, top and bottom no flow boundaries Variant B2-B5: Between 3.8 to 5.0 E5 Pa on all sides.	Hydrostatic head at infinite distance
Transmissivity(T) or conductivity(K) of feature A Standard deviation(SD)	At borehole sections: T=9.75E-9 – 5E-2 m^2/s from drawdown. Spatial distribution based on kriging	Not used. Radial steady-state flow field from pumping of 15 ml/min in KXTT3	RC-Test: T=4.9E-7 m^2/s	RC-Test: T=1.1E-7 m^2/s DP-Test: T= 1.25E-7 m^2/s DP-Test: Connective feature between KXTT2 and KXTT3 T=3.16E-5 m^2/s	Conductance of channels in Feature A: mean value = 1.8 m^2/year SD = 0.8 (log10)	mean T= 2.1E-7 m^2/s (mean log T=-6.67), SD = 1.0, T=3E-5 m^2/s 0.3 metres around borehole	RC-test: K = 3E-4 m/s DP-test: Mesh 1:As RC but K=1.5E-4 m/s near KXTT3 Mesh 2: Variable conductivity near boreholes between 1E-6 - 6E-4 m/s	RC-Test, Case 1: mean T= 5E-7 m^2/s (mean log T=-6.3) Cases 2&3: mean T= 3.2E-8 m^2/s (mean log T=-7.5) SD= 0.63 DP-Test, Case 1: T = 4.9E-7 m^2/s Case 2: mean T=2E-8 m2/s (mean log T= -7.7) SD = 0.63	mean T= 7.3E-7 m^2/s (mean log T=-6.1) SD=0.63	Mean T=4E-8 m^2/s (mean log T=-7.4)
Fracture aperture(FA) Flow porosity(FP) Effective porosity(EP)	Best fit for RC-1: FA=0.33 mm Best fit for DP-1 to DP-4: FA=0.23-0.75 mm	FA=1.4 mm FP=1	FA=1.4 mm FP=50%	RC-Test: FA=0.17 mm DP-Test: FA=0.178 mm DP-test: Connective feature between KXTT2 and KXTT3 FA= 2.82 mm	Aperture of channels from assumption that channel conductance is proportional to cubed aperture. Total channel volume of Feature A matches a flow porosity(FP) of 0.0008	Hydraulic aperture calculated using the cubic law on the local transmissivity. The ratio between transport and hydraulic hydraulic apertures was calibrated to about 15	FA = 1.4 mm (partly 0.8mm) EP = 0.3-0.4	RC-Test: Case1: FA=1.2 mm Case2: FA=0.16 mm Case3: 0.21 mm DP-test: Case1: FA=1.4 mm Case2 FA=0.18 mm	Equivalent FA = 0.096 mm mean log FA= -4.02 SD = 0.21	Equivalent FA: FA = 1 mm
Dispersivity Longitudinal (DL) Transversal(DT)	RC-Test: DL=0.19 m DP-Test: DL=0.71-1.37 m Ratio DL/DT=10	DL=0.5-0.55 m	DL= 0.55 m DT= 0.05 m	DL = 0.6 m DT = 0.06 m	Hydrodynamic dispersion modelled explicitly by hetereogeneous flow field.	Hydrodynamic dispersion modelled explicitly by hetereogeneous flow field.	DL = 0.6 m DT = 0.12 m	Hydrodynamic dispersion modelled explicitly by hetereogeneous flow field.	Taylor dispersion	DL=30 cm(case1) DL=60 cm(case2)
Correlation length for T	1 m	Not used	Not used	Not used	Channel conductance not correlated in space.	0.4 m	Not used	1 m	0.4 m	Not used

The deterministic homogeneous models (PNC/Golder: SEEP/W, BMBF/BGR: Mesh 1, SKB/KTH-TRUE: unconditional) have used a transmissivity corresponding to that which can be derived from the preliminary tracer experiment ($5 \cdot 10^{-7}$ m^2/s). However, in the PNC/Golder DFN-model a somewhat lower value was used ($1.1 \cdot 10^{-7}$ and $1.25 \cdot 10^{-7}$ m^2/s in the RC and DP test, respectively) based on an analysis of the flow logging in the boreholes from Dershowitz et al. (1996). For the simulations of the dipole test, the BMBF/BGR team calibrated the hydraulic conductivity in the areas around the boreholes to fit the measured drawdown in the radially converging test 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 teams using stochastic continuum models (Posiva/VTT and SKB/KTH-TRUE) have used information from the pressure build-up tests and the interference test with the source in KXTT3. The Posiva/VTT team started using the transmissivity distribution calculated from the pressure build-up test ($\log_{10}$ of the transmissivity with a mean, m_Y, of -7.4 and a standard deviation of 0.63). However, they found that the measured drawdown in the preliminary tracer test could be better simulated using a higher mean of the $\log_{10}$ of the transmissivity ($m_Y = -6.67$), more similar to what was found in the interference test, and a standard deviation of 1.0. 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 value of 1.0. No conditioning of the transmissivity field to the measured borehole transmissivities was made.

The SKB/KTH-TRUE team used several approaches for generating the transmissivity field testing different methods for conditioning. The mean transmissivity used in the unconditional case was taken from the interpretation of the preliminary tracer test (m_Y=-6.3). The mean value used as input for the conditional cases was taken as the geometric mean of the transmissivity of the borehole sections (m_Y=-7.7) estimated from the pressure response in the interference test. The estimations of transmissivity from the interference test were different from those given in Winberg (1996) due to a different evaluation model. In the simulations of the radially converging case the transmissivities of two of the sections were taken from the pressure build-up tests, which resulted in a slightly higher mean. For all cases a variance derived from the transmissivity of the borehole sections (σ^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 $1.4 \cdot 10^{-7}$ m^2/s.

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 team used a correlation length of 1 m in their base cases.

The fracture aperture used in the deterministic homogeneous models is generally based on the effective fracture aperture evaluated from the preliminary tracer experiment (b=1.4 mm). In some cases (PNC/Golder SEEP/W, BMBF/BGR) a reduced fracture porosity was used. The PNC/Golder DFN-model used transport apertures based on the transmissivity using an empirical relationship (Uchida et al., 1994). In the stochastic continuum models used by the SKB/KTH-TRUE team a constant fracture aperture was calibrated against the mean travel time of the preliminary tracer test for the simulations of the radially converging test. For the simulations of the dipole tests the aperture was calibrated against the mean travel time of the radially converging test. The Posiva/VTT team used a variable hydraulic aperture derived from the local transmissivity using the cubic law. However, to correctly simulate the breakthrough curves from previous experiments a local transport aperture about 15 times higher than the hydraulic aperture was used.

The transport models based on the advection-dispersion model have used a longitudinal dispersivity similar to that obtained from the evaluation of the preliminary tracer experiment (D_L=0.6 m). However, the evaluated dispersivity from the same configuration in the radially converging test and dipole test was lower (D_L=0.24 m and 0.4 m, respectively). Calibration of the dispersivity was made to a very limited extent.

5.4 Boundary conditions

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. However, different methods were used to assign the fixed heads on the boundaries, generally as hydrostatic heads or by extrapolating heads measured in the boreholes before the experiment out to the boundaries. However, the extrapolation of heads is not a straightforward procedure. For example, the extrapolated heads may be invalid if there are well conducting fractures intersecting Feature A close to the boreholes. Furthermore, measurements of head in the borehole sections before the preliminary tracer test, before the radially converging test and before the dipole test show that the background head field is slowly changing over time. The heads have decreased by about 7 meters over a period of nine months. Also the direction of the average gradient has changed over time from KXTT4 towards KXTT3 before the preliminary experiment to go from KXTT3 towards KXTT1 before the radially converging test, the latter more consistent with the existence of the tunnel.

Several of the modelling groups have used different boundary conditions in their simulations. The PNC/Golder team investigated four types of boundary conditions (Section 3.2.3) and found large differences in the direction of transport and mass recovery. They concluded that the point dilution method gave the most likely interpretation of the head field during the experiment. The SKB/KTH-TRUE team performed calculations where the head values on the boundaries were perturbed in the conditioning. The additional freedom of having fluctuating boundary conditions resulted in a smaller variance of the transmissivity field after conditioning.

5.5 Model calibration and conditioning

The modelling teams initially received data deliveries (Data delivery No 1 - 4 for Task 4C) containing information from the site characterisation and the design of the radially converging tests, cf. Section 2.2.3. After the model predictions of the radially converging tests were made the experimental data were revealed in Data delivery No 5 for Task 4C. This information together with test design for the dipole tests (Data delivery 1 for Task 4D) was available for the modelling teams in their predictions of the dipole tests. Finally, after the model predictions of Task 4D were made the experimental results were revealed in Data delivery No 2 of Task 4D. A summary of the modelling team's usage of the delivered data is given in Table 5-2. The modelling teams were also asked to indicate the importance of various data for setting up their model and for estimation of model parameters.

The methods for using the additional data obtained in the series of experiments performed in Feature A have varied from direct calibration of the model parameters to a more complex conditioning of transmissivity fields based on measured transmissivities and head values.

Modelling of the radially converging test is based on site characterisation data and the result of the preliminary tracer test. However, there was considerable uncertainty in these data, e.g. there are large variations in the transmissivity values evaluated from the different tests. Most of the modelling teams based their predictions of the radially converging test on a model calibrated on the preliminary tracer test.

The predictions of the radially converging tracer test, partly with the same geometrical configuration as the preliminary test, showed a high accuracy in the prediction of tracer breakthrough time from the two closest injection points. However, the majority of models could not predict the limited mass recovery from the two injection points further away obtained in the experiment. The predicted drawdown was far from the experimental results.

The results of the radially converging experiments were made available for the predictions of the dipole tests and could be used for calibration and conditioning. All teams have adjusted the hydrological parameters such as transmissivity or conductivity, and most of the teams have made adjustments of transport parameters such as fracture aperture or flow porosity. A reasonable accuracy was obtained for the predictions of the tracer breakthrough time. The predictions of breakthrough time for the dipole DP-1, with an equivalent configuration as used in one of the radially converging tests, showed a decrease in accuracy in the predictions of breakthrough time. However, there were considerable improvements in the predictions of mass recovery and also in the prediction of drawdown in the borehole used as pumping hole in the radially converging experiment. However, the drawdown observed in the other boreholes was not predicted with any greater accuracy.

There are several factors that have contributed to the difficulties in performing the predictive calculations:

- The long source term duration in the preliminary tracer test and the radially converging test in comparison with the travel time concealed much of the details of the transport in the fracture, e.g. the presence of separate flowpaths. The quality of the information that could be obtained from these tests was therefore limited.
- The use of the radially converging test as a basis for calibration was somewhat limited due to the lack of recovery from the injection points in KXTT2 and KA3005A. Only the tracer tests with injections in KXTT1 and KXTT4 could be used for subsequent calibration. The lack of recovery from KXTT2 was in contrast with the large drawdown response observed in KXTT2.
- Drawdown is to a large extent dependent on the local transmissivity close to the borehole section, particularly for pumping holes and forced injection holes. Thus, homogeneous models are not able to correctly describe this, and for stochastic continuum models not conditioned to measured data there will be large variations between individual realisations.
- Local gradients cannot be accurately estimated due to the influence of connecting features.
- The background head field (magnitude and direction of gradient) has slowly changed during the series of tests.

A problem many of the modelling teams have experienced is how to find a suitable relationship between the fracture aperture derived from the hydrological tests (hydraulic aperture) and that derived from the tracer experiments (transport aperture or mass balance aperture). This is needed in order to correctly model both drawdown and tracer breakthrough. The modelling teams have dealt with this by independent calibration of a transport aperture or by introducing scaling relationships between transmissivity and transport aperture. However, such relationships are likely to be very site specific and will thus have limited predictive capabilities if applied to other sites. Further studies of the effect of variance of fracture transmissivity and fracture aperture will be helpful in increasing the understanding of this subject, e.g. TRUE-1 Pilot Resin Experiment and planned resin injection and excavation of the TRUE-1 site.

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

Modelling group Task	CRIEPI 4C 4D	PNC/Golder 4C 4D	SKB/KTH-ChE 4C 4D	Posiva/VTT 4C 4D	BMBF/BGR 4C 4D	SKB/KTH TRUE 4C 4D
Data delivery No 1 for TASK No 4C 1996-02-15 and Data delivery No 2 for TASK No 4C 1996-03-04:						
Descriptive Stuctural-hydraulic models on Block and detailed scales (Winberg A., 1996)	M M	P P	P	P P	X X	M M
Borehole deviation data Appendix A	- -	p p	X	- -	X X	P P
Pressure data from the pressure build-up tests	- -	m m	X	- -	m m	X -
Flowdata from the pressure build-up tests	- -	m m	X	m m	m m	X -
Transmissivities evaluated from pressure build-up test	P P	P P	X	P P	X X	p -
Data from single packer flow logging	- -	P P	X	m m	X X	X -
Transmissivities evaluated from flow logging	- -	P P	p	P P	X X	m -
Pressure data from the interference tests(Data Delivery 2)	- -	p p	X	m m	X X	P P
Drawdown and recovery data from the interference test	- -	p p	X	m m	P P	P P
Transmissivities evaluated from interference test	- -	P P	X	P P	X X	- -
Data from the preliminary tracer tests	- -	P P	P	P p	P p	P -
Evaluated material properties from preliminary tracer tests	- -	P P	p	M M	X X	M M
Measured pressure and hydraulic head	- -	P P	P	P p	P P	p -
Tracer dilution tests	- -	p p	X	P p	P	- -
Data delivery No 3 for Task No 4C 1996-04-15:						
Experimental data for RC-1, pumping rate and injection concentration as a function of time	P -	P	P	P -	P P	P -
Data delivery No 4 for Task No 4C 1996-04-19:						
Discrete Fracture Analysis in Support of the Äspö Tracer Retention Understanding experiment (TRUE-1), (Dershowitz W., 1996)	- -	P P	m	m m	X X	- -
Data delivery No 5 for Task No 4C 1996-10-22						
Injection concentration and pumping rate versus time for RC-tests	P -	P P	P	P -	P P	- -
Breakthrough concentration versus time for RC-tests	P -	P P	P	X -	P	- p
Head data for RC-tests	P -	P P	P	- p	P P	- P
Sampling flow rates for RC-tests	P -	P P	p	P -	P P	p -
Data delivery No 1 for Task No 4D 1996-11-14:						
Pumping rate and the injection concentration versus time for DP-tests	- P	p P	P	- P	P	- P
Tracer test design for the TRUE-1 dipole tests.	- M	p P	P	- P	P	- P
Experimental data and preliminary evaluation of the TRUE-1 RC-1 Test (HRL-96-24)						
Tracer breakthrough data interpretation	m -	P	X	- m	P	M M
Numerical modelling	m m	m	X	- -	X	- -
Hydraulic head distribution	m -	P	X	- M	P	m m
Hydraulic head response in adjacent sections	- -	P	X	- m	P	m m
Electrical conductivity and water chemistry	- -	m	-	- -	p	- -
Data delivery No 2 for Task No 4D 1997-03-14:						
Breakthrough curves for DP-tests	- P		P	- X	P	- -
Injection curves for DP-tests	- P	P	P	- P	P	- -
Head data for DP-tests	- P	P	P	- P	P	- -
Pumping rate data for DP-tests	- p	P	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

5.6 Sensitivity analysis

The different modelling groups have performed a sensitivity analysis of their models either by variations in the models or by variations of the input parameters. Sensitivity analysis has been performed in the following areas:

- discretisation of Feature A used in the model

- transmissivity or transmissivity distribution

- boundary conditions

- transport porosity or transport aperture

The modelling groups (CRIEPI, SKB/KTH-ChE, Posiva/VTT, BMBF/BGR and SKB/KTH-TRUE) that have studied the effect of discretisation found only minor changes in the results using a finer mesh than used in the base case. The changes were primarily noticable for the transport calculations. The SKB/KTH-TRUE team found that the mean travel time in the radial converging experiment increased about 60% when using elements one half of the original size. This may be caused by the same calibrated transport aperture being used for both cases. However, it is hypothesised that the finer discretisation gives an increased flow path heterogeneity that results in longer travel times. A sufficiently small discretisation is particularly important to describe the small scale variability when using a short correlation length. In the models using a stochastic field for the transmissivity (Posiva/VTT and SKB/KTH-TRUE), the element size in the different simulations has varied between 0.12 and 0.8 times the correlation length. The transmissivity fields generated with an element size in the upper range were inadequate to describe the correlation structure. This resulted in a high variance in the transmissivity field for these simulations and a high uncertainty in the predicted drawdown.

The modelling teams have performed variations of the transmissivity in Feature A as a part of the model calibration. The transmissivity, or the mean value of the transmissivity distribution in case a stochastic distribution was used, has a strong influence on the predicted drawdown. However, the effect on breakthrough times was considerably less because of the constant rate pumping used in the experiments. The Posiva/VTT team concluded that the drawdown appeared not to be sensitive to the variance of the transmissivity field, but the corresponding transport time was. They further concluded that the mean transmissivity has a strong influence on the recovery obtained in the tracer experiments. The SKB/KTH-TRUE team has performed various types of conditioning of the transmissivity field on head values from previous tests. The conditioned fields have ensemble statistics that deviate from the input statistics, most likely caused by the head conditioning introducing additional spatial variability.

Only the SKB/KTH-TRUE team varied the correlation length. They concluded that a reduced correlation length gave higher uncertainty in drawdown due to increased transmissivity variance.

The variations of the boundary conditions performed by the PNC/Golder team indicate the importance of the boundary conditions for drawdown and mass recovery. Allowing for fluctuating boundary conditions in conditioning of the transmissivity field made by the SKB/KTH-TRUE team, results in smaller transmissivity variability. This gives a minimal effect on the uncertainty in drawdown, but results in a reduction of uncertainty in the transport estimates.

Concerning the transport parameters most of the modelling teams performed a variation of the fracture aperture or flow porosity as a part of the calibration. As can be expected the breakthrough times were directly related to the fracture aperture.

5.7 Lessons learned - Unresolved issues

Experimental site characterisation

The characterisation of the experimental site was generally thought to be good. Areas where an increased understanding was considered necessary were the characterisation of the head field, the boundary conditions and the connectivity structure, especially the existence of bypassing features needs to be examined.

The presentation of the characterisation data could be improved. The data were not given in a collected form, but mixed with conceptual models and other information.

Experimental design

The long source term of the radially converging experiment reduced the potential for analysing relevant transport processes when interpreting the breakthrough curve. A shorter, better defined and measured source term was considered essential. The problem with the long source term was corrected for the dipole tests. Furthermore, uncertainty in the input flux could be reduced by a better control of the injected mass flux. Development of injection methods was therefore concluded to be an important task, and consequently improved injection methods have been developed for the subsequent tracer tests in Tasks 4E and 4F.

Performance measures

The performance measures for mass recovery and mean breakthrough time are fundamental measures describing the quality of the predicitions. However, performance measures based on long lasting injection curves are unsuitable, e.g. t50 or t95 of the whole injection curve. Due to the short travel times of the experiments and the slow decay of the injection curve, the time to recover 5, 50 or 95% has almost the same meaning. The inclusion of the mean tracer travel time, as was done for Task 4D is essential since it is an important entity in tracer tests.

The definition of the accuracy measure, cf. Section 4.3.1, should be revised. With the present definition 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. An alternative would be to use the logarithm of the ratio between the predicted and the measured value.

It would be more useful to give the measure for spread in time, ($D_t = t95 - t5$) normalised to *t50* rather than as absolute numbers, due to linear scaling with aperture, i.e. $D_t = (t95 - t5)/t50$. Mass recovery is important for understanding the existence of multiple pathways. In TRUE-1 mass recoveries were given for specified times, which confuses with transport time. Projected ultimate mass recovery could be an additional performance measure.

Suggestions for additional data and analysis

In their response to the questionnaire the modelling groups have several suggestions for additional data that may be required to make a more reliable prediction of the tracer experiments:

- The PNC/Golder team advocated the need to use all available data in setting up the model. Specifically, they proposed a more detailed analysis of performed interference tests that would be helpful in defining a structural/ hydraulic connectivity model for Feature A. Furthermore, additional analysis of transient hydraulic responses in injection/pumping intervals would increase the understanding of transmissivity structure near wells. An understanding of the detailed internal structure of Feature A is important to understand the transport properties, such as the relationship between transmissivity and transport aperture. For the subsequent tests with sorbing tracers also data on the flow wetted surface and fracture mineralogy is important.

- Increased understanding of the boundary conditions was considered important by the SKB/KTH-ChE and SKB/KTH-TRUE teams. More head measurements at different locations in the rock mass to improve the knowledge of the boundary conditions were proposed.

- The POSIVA/VTT team pointed on the need to perform thorough flow measurements based on tracer dilution of both background flow field and flow field during pumping. This has since been implemented for the TRUE-1 tracer tests. POSIVA/VTT also proposed measurements of flow rate distributions in the fracture also in various scales, e.g. in boreholes intersecting the fracture close to each other (20-50 cm).

- The modelling teams using stochastic continuum models (CRIEPI, PNC/Golder, SKB/KTH-TRUE, Nirex/AEA) stressed the need for spatial distribution of aperture in Feature A, as will be obtained from the resin experiment. Furthermore, increased knowledge on the relationships between transmissivity, storativity, transport aperture and fracture roughness was considered important.

- The BGR/BMBF team had suggestions aiming at a better knowledge of the tracer plume. In the case of low recovery, additional measurement of the concentration in the other boreholes and / or in the interval of Feature B could be performed to obtain more detailed information about tracer distribution in the fracture system.

Additional generic research required.

The modelling teams have also identified areas where they consider additional research is required. One such important area is the effect of heterogeneous flow on the transport in a fracture including topics such as:

- generic relationships between transmissivity, storativity, transport aperture and roughness which are needed in order to make predictions of transport without site-specific data from tracer tests,

- the nature of flow and transport at fracture intersections,

- the effects of mineralisations and fracture infillings,

- the relationship between dispersivity and spatial distribution of fracture aperture,

- information about the flow wetted surface, and how this entity is correlated with the water flow rate, which is important for modelling sorbing tracer transport.

6 Conclusions

6.1 Tasks 4C and 4D as a testing exercise

Modelling Task 4C was defined to perform predictive modelling of the radially converging tracer test in Feature A at the TRUE-1 site, including a comparison of model outputs with experimental results. The tracer test was preceded by a characterisation of the site and a preliminary tracer experiment. Modelling Task 4D comprised predictions of a sequence of dipole experiments performed using information from the previously performed tracer tests.

The modelling teams have performed an impressive amount of modelling considering the large amount of data available and the time constraints. Many of the modelling teams have tested alternative models for evaluating the effects of structural models, transport processes, boundary conditions and heterogeneity. In the work there has been considerable interaction between experimentalist and modellers, which is vital for setting up relevant experiments, for understanding the results and for performing relevant modelling.

The modelling performed within Task 4C and 4D is a good illustration of the complexity of making predictions of flow and transport in fractured rock. The results of the predictive modelling makes it evident that the boundary conditions, the flow system and its effect on the transport were not completely understood at the time of the experiment. Several hydraulic tests have been performed in Feature A, despite this the predicted drawdown in the radially converging test was generally far from the experimental results. The modelling teams had problems with overpredicting the drawdown in the radially converging experiment using transmissivities from the pressure build-up tests. The only models that were able to explain the low drawdown were the PNC/Golder discrete fracture model and the SKB/KTH-TRUE unconditional model. The PNC model uses a lower transmissivity, but has many intersecting fractures causing Feature A to behave as a leaky aquifer. The SKB/KTH-TRUE unconditional model uses a mean transmissivity derived from the preliminary tracer test, while the SKB/TRUE conditional models, that overpredicts the drawdown, used a mean transmissivity from the pressure build-up tests and interference tests.

Estimates of the transport parameters were available from the preliminary tracer experiments. The predictions of the radially converging tracer test, partly with the same geometrical configuration as the preliminary test, showed a high accuracy in the prediction of tracer breakthrough from the two closest injection points. However, the majority of models did not predict the lack of recovery from the two injection points further away. The lack of recovery from KXTT2 during the radially converging test, despite the large hydrological response from the pumping, is an example of the need for understanding of the heterogeneity of Feature A and the boundary conditions when making predictions of tracer tests.

In the predictions of the dipole tests, when the results of the radially converging experiments were made available and could be used for calibration and conditioning, a reasonable accuracy was obtained for the predictions of the tracer breakthrough. There were considerable improvements in the predictions of mass recovery and also in the prediction of drawdown in KXTT3, the borehole used as pumping hole in the radially converging experiment. However, the drawdown observed in the other boreholes was not predicted with any improved accuracy.

There are several factors that have contributed to the difficulties in performing the predictive calculations:

- the long source term used in the preliminary tracer test and the radially converging test reduced the potential for analysing relevant transport processes when interpreting the breakthrough curves.

- the lack of data concerning the head at the boundaries

- the slowly changing background head field during the series of experiments.

- the difficulty to simulate drawdown due to its sensitivity to local transmissivity.

One difficulty with tracer tests in low permeability features is to find an optimal relation between the pumping rate and the background gradient. A low pumping rate may lead to difficulties to recover tracers from the injection points, but gives a relatively undisturbed flow field and sufficiently long travel times to evaluate the breakthrough curve. High pumping rates give a better chance for tracer recovery, but will affect the flow field and may give too short travel times to reveal the characteristic transport processes.

6.2 Modelling and data

Although Feature A is not a simple unconnected structure, the predictive modelling shows that Feature A can be approximated as a singular well-connected feature with limited connectivity to its surroundings for predictions of drawdown in boreholes and conservative tracer breakthrough. Reasonable estimates can be obtained using simple models. However, more elaborate models with calibration or conditioning of transmissivities and transport apertures are required for more accurate predictions. The modelling work performed within these tasks also demonstrate the benefits of using several models based on different concepts and of varying complexity for predictions and evaluations. An example is the alternative models used by PNC/Golder and Posiva/VTT for evaluating certain important aspects concerning, e.g. boundary conditions and flow field distribution.

The modelling work has identified that the general processes are well understood, but the present understanding of the heterogeneity of the feature is limited and needs to be further evaluated. Measurements of the spatial aperture distribution are planned in the resin injection experiment. However, since this is a destructive test method it can only be performed after the tracer tests are completed. Additional flow measurements, e.g. measurements of flow rate distributions in closely spaced boreholes intersecting the feature, could give information of the heterogeneity in the flow field. Practically, this could only be performed in a limited domain of the feature.

A problem experienced by the modelling teams is how to find suitable relationships between the fracture aperture derived from the hydrological tests (hydraulic aperture) and that derived from the tracer experiments (transport aperture or mass balance aperture). This is needed in order to correctly model both drawdown and tracer breakthrough. The modelling teams have dealt with this by independent calibration of a transport aperture or by introducing scaling relationships between transmissivity and transport aperture. However, such relationships are likely to be very site specific and their use for predictive purposes needs to be further evaluated. Further studies of the effect of variance of fracture transmissivity and fracture aperture will be helpful in increasing the understanding of this subject.

Many of the modelling teams have stressed the importance of the boundary conditions applied at the model boundaries. The boundary conditions have generally been assigned by extrapolation of the measured heads in the boreholes. This gives rise to some uncertainty in the head field in the outer parts of the feature due to the effect of intersecting fractures. However, a sufficient understanding has been obtained of the part of Feature A encompassed by the triangle KXTT3-KXTT4-KXTT1. An increased knowledge of the boundary conditions in the outer parts of the feature could be obtained by additional measurements and/or by models covering a larger domain, e.g. fracture or channel network models or nested models.

The methodology to derive the necessary parameters for predictions needs development. The tracer tests were preceded by a site characterisation, including hydrological tests and a preliminary tracer experiment. However, the modelling teams have not used the data set from the site characterisation to its full extent for their predictive models (e.g. the interference tests and pressure build-up tests). Furthermore, there is a disparity among the modelling teams in their approach to assigning the material property values used in the models. This indicates the need for development of methods to make use of all data produced from the site characterisation in the modelling. The conditioning of the transmissivity field based on measured transmissivites and heads seems to be a promising methodology. Also the methods for the use of supplementary data, e.g. geophysical logs and hydrochemical data, needs developing. The integration of hydrological and hydrochemical information is an issue addressed by Task 5 of the Äspö Modelling Task Force.

6.3 Perspective to future tasks

The Modelling Tasks 4C and 4D focus on advective and dispersive transport of non-reactive tracers in low permeability fractures. The emphasis is on the effect of heterogeneity on the head field and the tracer time distribution. The advective and dispersive transport in low permeability features is an important issue in performance assessment. The transport of non-reactive tracers is largely determined by flow porosity, while this parameter has less importance for sorbing tracers. A problem experienced by many of the modelling teams is how to find generally applicable relationships between fracture transmissivity and transport aperture. In order to correctly predict both drawdown and tracer breakthrough time, the transport aperture had to be upscaled. In lack of generally applicable relationships between transmissivity and transport aperture, the approach presently used in performance assessment models of using a constant transport porosity set at a low value can be justified.

Good knowledge of the hydraulic and transport properties of the studied feature is needed for the understanding of the important transport mechanisms and for setting up and evaluating tracer experiments. The radially converging and dipole tracer experiments and the associated modelling work have increased the understanding of the flow and transport in Feature A and have contributed valuable knowledge and experience for the subsequent experiments within TRUE-1 with sorbing tracers. Predictive modelling of the TRUE-1 experiments with sorbing tracers is performed within Tasks 4E and 4F. The subsequent experimental work within TRUE-1 and modelling work within Task 4 has shown that a sufficient understanding has been obtained of the part of Feature A encompassed by the triangle KXTT3-KXTT4-KXTT1.

As a result of their work, the modelling teams have several suggestions for investigations giving additional data that would give better defined tracer experiments and more reliable predictions. This includes further analysis of the tests performed within the site characterisation as well as further measurements of the head distribution and the flow distribution. These suggestions have been helpful in designing the sorbing tracer experiments performed within TRUE.

The transport of sorbing tracers is greatly influenced by mass-transfer, whereby additional properties of the feature are of importance, e.g. the flow wetted surface, and the diffusion and sorption properties of the rock. Since many important radionuclides in a repository for spent nuclear fuel to some extent are sorbing, the work within these modelling tasks will be of great importance for the performance assessment.

7 Acknowledgements

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Appendix 1 Data distributed

Task 4C: Data distribution 1 to 5:

Data delivery No 1 for Task No 4C:

- Report "Descriptive Structural-Hydraulic Models on Block and Detailed Scales" Final Draft version.
- Performance measures and presentations formats.
- Report on the TRUE-1 tracer test programme valid for Task No 4C

Data delivery No 2 for Task No 4C:

- Disk 1:

Borehole deviation data
Pressure data from the pressure build-up tests
Flow data from the pressure build-up tests
Data from single packer flow logging

- Disk 2:

Pressure data from the interference tests

- Disk 3:

Drawdown and recovery data from the interference tests

- Disk 4:

Data from preliminary tracer tests

Data delivery No 3 for Task No 4C:

- Complementary experimental data of RC-1. Information regarding pumping rate and injection concentration as a function of time.

- Some clarifications of the geometry of 3rd order zones NW-2 and NW-3.

Data delivery No 4 for Task No 4C:

- The FINAL DRAFT version of "Descriptive Structural-hydraulic Models on Block and Detailed Scales"

Data delivery No 5 for Task No 4C:

- Injection concentration (ppm) versus time (h) of:
  Uranine (KXTT1 R2)
  Rhodamine WT (KXTT2 R2)

Amino G	(KXTT4 R3)
Eosin Y	(KA3005A R3)

- Breakthrough concentration (ppb) versus time (h) for Uranine, Amino G, Rhodamine WT, Eosin Y.

- Head data (metres above sea level) for KXTT1 R2, KXTT2 R2, KXTT2 R2, KXTT4 R3, KA3005A R3.

- Complete data set on pump flow rate (l/min) and electrical conductivity (mS/m).

Task 4D: Data distribution 1 to 2:

<u>Data delivery No 1 for Task No 4D:</u>

- Complementary information for the DP tests. Pumping rate and the injection concentration (ppm) as a function of time (h).

- Performance measures and presentation formats.

- A report on the test design for the TRUE-1 dipole tests #1-4

<u>Data delivery No 2 for Task No 4D:</u>

- Breakthrough curves:
  Breakthrough concentration (ppm) versus time (min) for:
  DP-1: Uranine in KXTT3 R2 from injection in KXTT1 R2
  DP-2: Amino G in KXTT1 R2 from injection in KXTT2 R2
  DP-3: Uranine in KXTT1 R2 from injection in KXTT2 R2
  DP-4: Amino G in KXTT4 R3 from injection in KXTT2 R2

- Pump flow rate and electrical conductivity of pumped water

Pumping rate (l/min) and electrical conductivity (mS/m) versus time for water pump during DP-1 – DP-4.

- Head Data:

Hydraulic head versus time for KXTT1 R2, KXTT2 R2, KXTT3 R2, KXTT4 R3, KA3005A R3 during DP-1 – DP-4

- Log of events

Appendix 2 Executive summaries

CRIEPI: SUMMARY AND CONCLUSIONS

The Tracer Retention Understanding Experiments (TRUE) (Olsson and Winberg 1997) consists of a planned series of tracer test cycles on different experimental length scales at the Hard Rock Laboratory, Äspö. The modelling of the outcome of the ***first*** tracer test cycle (TRUE-1) will be the subject of this report. The TRUE-1 experimental test cycle consists of performing tracer tests on a detailed scale in a simple test geometry. The calculations presented in this report correspond to a series of radially convergent tracer tests (RC-1) performed between an array of five boreholes spaced between boreholes 5.03m and 9.5m apart in a fracture called Feature *A*.

This report considers groundwater flow and dispersion of a non-reactive tracer in a single, heterogeneous feature. The spatial distribution of fracture aperture has been modelled as a two-dimensional stochastic process. The stochastic properties have been based on interpreted or measured values of transmissivity and hydraulic head. For the purpose of the calculations presented in this report it is assumed that the fracture aperture has a log-normal distribution - although there is no direct site-specific evidence for this being an appropriate model. For a smoothly varying aperture, the Navier-Stokes equations governing the flow in the fracture can be simplified substantially. A series of pathline calculations have been performed, based on one-hundred stochastic realisations for each set of parameters, to estimate the spread in the advective component of the flow. For each pathline an advection-dispersion equation based on Taylor dispersion was solved on the resulting one-dimensional stream tubes.

The modelling has explored the consequences of a simple variable aperture conceptual model for an isolated fracture. It begins with the premise that we understand the physics of laminar fluid flow and questions our only other freedom (for a non-reactive tracer) - geometry.

A preliminary tracer test was performed between boreholes KXTT-3 and KXTT-1 at the TRUE-1 site to complement the hydraulic information gathered as part of the initial characterisation of Feature *A*. Unfortunately, the preliminary tracer test revealed little of the details of flow in the fracture, as it was shown to be dominated by the characteristic shape of the source decay. Hence, this pre-test did not reveal much useful information pertaining to the transport characteristics of the fracture.

However, early indications indicate the experimentally measured travel times and apparent dispersion characteristics appear to be at significant variance with those likely to arise from the numerical models. This therefore is the first indication of the inadequacy of the underlying conceptual model of Feature *A*.

As the predicted travel times appear to be too short, the models require more resistance of the groundwater flow without substantially changing the flow volume. This can introduced by either incorporating large surface roughness or (and) multiple fractures that are in substantial contact. Within the existing conceptual model, very large variance of fracture aperture on a small length scale would be needed to increase the travel time form injection to recovery whilst maintaining the voidage of the fracture. This possibility should be explored in future work.

An alternative phenomenological approach would be to introduce the standard concept of fracture porosity and dispersion length or alternatively introduce scaling relationships between transmissivity and 'transport' aperture. However, this does not give any true insight into how flow and transport occur in a fracture and hence does not have true predictive capabilities.

SKB/KTH-CHE: SUMMARY

The TRUE project (Tracer Retention Understanding Experiments) comprises of a series of flow and transport experiments performed at different scales. The goal of these tracer tests was to develop a better understanding of radionuclide migration and retention in fractured rock.

The first stage of the TRUE project at Äspö involved interference tests, dilution tests, flow logging, pressure build-up tests and preliminary tracer tests. After this, the radially converging tracer test (RC-1) in Feature A was performed with steady-state water extraction in KXTT3. This was followed by a dipole experiment including four tests (DP 1-4). From the field studies, Feature A seems to be a single Feature with possible intersections with other fractures.

In the modelling of the TRUE experiments the codes CHAN3D-flow and CHAN3D-transport, which are both based on the Channel Network model, were used. Initially, the geometric information and boundary conditions were inserted to the flow model and the resulting flow distribution was then used in the transport model.

The tasks 4C and 4D comprised of blind predictions of these tracer tests. For the radially converging tracer test, information from a preliminary tracer test in Feature A was available, in addition to the geometric and hydraulic data. For the dipole tracer tests information of the RC-1 test was available.

RC-1 was performed in a radially converging flow geometry with water withdrawal from KXTT3-R2. Injection of tracers was performed on all other borehole sections that penetrated Feature A; KXTT1-R2, KXTT2-R2, KXTT4-R3 and KA3005-R3. This geometry implied travel distances between 4.7 to 9.6 m. The dipole tests were performed once between KXTT1-R2 and KXTT3-R2, twice between KXTT2-R2 and KXTT1-R2 and once between KXTT2-R2 and KXTT4-R3.

In general the predicted results agreed well with the experimental results. Difficulties were observed in the prediction of the drawdown in the injection and extraction sections of the dipole experiment, since no conditioning was done in these regions.

To limit the water flow into the tunnel, the skin effect was introduced. It was observed that when the value of the factor that takes into account the skin effect is too small, most of the tracer injected was transported into the tunnel.

POSIVA/VTT: EXECUTIVE SUMMARY

First phase of the TRUE (Tracer Retention Understanding Experiments) is ongoing in the Hard Rock Laboratory at Äspö. The first phase of the project includes tracer tests in a simple flow geometry and small scale. The length scale of the experiments is from four to ten metres.

The target feature used for the experiment was selected after a thorough testing of the site. Four possible features were initially found. The selected one, feature A, was the best defined and hydraulically rather isolated. Also, the transmissivity of that feature was of the right order of magnitude. Other features were very complex and more connected to the surroundings.

Five boreholes were drilled through the feature A. In the radially converging test all of the boreholes were used by pumping one of them and injecting from the rest of the boreholes. In the dipole tests only four boreholes were used.

The experiments were performed in a stationary flow field. In the case of the radially converging experiment the target fracture was pumped for one week prior to the experiment. For the dipole experiments the pumping times were somewhat shorter, a couple of days. The tracer experiments were performed using nonsorbing tracers and decaying pulse injection.

The radially converging tracer test resulted in high recovery from two of the boreholes closest to the pumping hole, but no recovery from the two of the furthest boreholes. Transport distances from the closest boreholes was about 5 metres and from the furthest ones about 10 metres. It was assumed that the low recovery from the furthest boreholes was due to a leak into the feature A. The radially converging tracer test did show a modest dispersion during the transport and the breakthrough curves were dominated by the long tailing of the source terms. The time resolution in the experiment was not high enough to determine accurately the dispersion.

In the dipole tests recovery was obtained in all of the experiments. The dipole experiments showed larger drawdowns than were expected and the dispersion was significantly higher in the dipole experiments than in the radial experiments.

Predicting the radial tracer test succeeded better than the dipole experiments. This is understandable because the transport aperture in the radial test was calibrated against the preliminary tracer test. The only difference between the preliminary tracer test and the radially converging tracer test was the different pumping rate. On the other hand, the quite long tailing in the source term of the radial experiment was dominating in the breakthrough and had a consequence that all the predictions were more or less similar in the overall behaviour.

In the dipole tests the predictions presented in this report showed too low drawdowns and too long transport times. This might result from slightly biased transmissivity field

applied in the model. Also, the transmissivity field used in the simulations was not conditioned to the measured transmissivities of the injection and pumping holes.

Both the measured and numerically simulated results were compared against the one-dimensional advection-dispersion model. The results indicate that the dispersion in the radial experiment was quite low. In the dipole experiments the dispersion was significantly higher. Reason for this might be that the dipole test activates more probably several separate flow paths whereas the radial flow field is favouring a single flowpath. Therefore, it can be thought that the difference between the dipole and radial tests is similar with the corresponding change in the size of the source. In the radial test the source was practically a point source as in the dipole tests the source is much more spread. The simulated dispersivities were in all cases smaller than the measured ones.

BMBF/BGR: EXECUTIVE SUMMARY

The Federal Institute for Geosciences and Natural Resources (Bundesanstalt für Geowissenschaften und Rohstoffe, BGR), supported by Federal Minister for Education, Sciences, Research and Technology (Bundesministerium für Bildung, Wissenschaft, Forschung und Technologie, BMBF) began a program in the Äspö Hard Rock Laboratory (Sweden) in 1995 to characterize sites for the disposal of high-level radioactive waste in granite. This program comprises two parts: modelling of groundwater flow and transport of solutes (TRUE Experiments) and study of two-phase flow.

During the last four phases (1984 – 1997) of the research work at the Grimsel Test Site, a numerical program system, DURST/Rockflow, based on the finite-element method was developed jointly by BGR and the Institute of Fluid Mechanics of the University of Hannover to simulate flow and solute transport in fracture systems. This program system has been successfully used to study the hydraulic tests and tracer experiments in the Grimsel Rock Laboratory.

To test the suitability of the developed methods and numerical models for water-saturated rock formations, especially for those at Äspö, two models SM2 (flow model) and TM2 (transport model) have been applied to interpret the experimental results within the scope of the modelling of the radially converging tracer tests (TRUE-4C) and dipole tracer tests (TRUE-4D).

At the beginning of the modelling, a homogenous model with two coupled fracture systems, Features A and B, was used based on relatively little geometric and hydrogeological information. This model was calibrated with the data obtained from measurements of the natural flow system and the preliminary tracer test. To some extent, study of transport parameters, e.g., effective porosity, dispersivity, and diffusion coefficients, has eliminated uncertainties in the values of the transport parameters of the numerical model. However, the complex flow geometry could not be interpreted correctly in the first stage. The calculated hydraulic head in the fracture systems showed that the hydraulic influence of Feature B on Feature A could be neglected when the experimental configurations in the 4C and 4D tests were used. Therefore, in the subsequent modelling, only the hydraulic properties in Feature A were given close attention.

The fracture model of Feature A was modified after the publication of the data from the radially converging tests. Two different meshes with variable hydraulic conductivity and fracture aperture were set up according to different calibration criteria. For the first mesh, the difference in pressure between the injection and pumping boreholes (KXTT1 and KXTT3) and the tracer breakthrough time in the radially converging test were used as criteria for model calibration. In the second case, the fitting of the hydraulic drawdown from the modelling results to the measurements in all five boreholes from the radially converging test was given more attention. These two meshes yielded a quite inhomogeneous fracture model. However, the drawdown near borehole KXTT2:R2 could not be modeled exactly due to the complicated geometry there. From our experience gained from the in situ experiments at Grimsel Test site, channeling must occur between boreholes KXTT3 and KXTT2 besides the planar fracture system.

The results of the predictive calculations for the dipole tests show that a satisfactory tracer arrival time and breakthrough curve are obtained with both meshes, even though the measured and modeled drawdown are quite different. The results with the second mesh fit the measured data better than those with the first mesh, especially in dipole tests DP2 and DP3 from KXTT2 to KXTT1, which are only 2.59 m apart. It indicated that the non-homogenous model can better describe the natural fracture system and corresponding boundary conditions. But both meshes should be modified further when more test data is known.

Tracer migration is affected more by advection than by diffusion, especially at short distances of 5 – 10 m. Thus it is very important to determine the flow field correctly. In the large-scale tracer experiment, diffusion capacity of the rock should be taken into consideration in order to model tracer transport reasonably. The longer "tailing" in the breakthrough curve in a large-scale tracer test of more than 100 m, in Grimsel rock laboratory can be explained by channeling and diffusion in the fractured rock.

The modelling of flow and tracer transport in the small-scale experiment serves to verify the conceptual method and numerical model and to determine the transport parameters using the data from in situ experiments. With a confirmed method and verified model, the groundwater and solute transport problem can then be solved numerically.

SKB/KTH-TRUE: EXECUTIVE SUMMARY

The report summarizes modelling work performed within the First Stage of the Tracer Retention Understanding Experiments (TRUE). Specifically the report presents and discusses predictions of non-sorbing tracer tests in Feature A of the TRUE-1 site. These predictions are the contribution of the SKB/TRUE Modelling Team to Tasks 4C and 4D of the SKB Task Force on Modelling of Groundwater Flow and Transport of Solutes. Task 4C deals with a radially converging experiment whereas Task 4D deals with dipole experiments. The overall objective of the present study is to compile the results produced within Tasks 4C and 4D, and to increase the level of understanding of the studied feature by means of various complimentary analyses utilizing the previously used numerical tools and some simple back-of-the-envelope tools.

A two-dimensional stochastic continuum description of the feature is adopted. Monte Carlo realizations provide a means for assessing the uncertainty in the predictions. Both unconditional and conditional generators for the underlying spatially variable transmissivity fields are used. The conditional simulations utilize measured data of both transmissivity and steady-state head values. Five values of transmissivity are used. For steady-state head, five values prior to pumping or five values prior to pumping and during pumping are used.

The flow problem is solved using a mixed hybrid finite element formulation. A Lagrangian travel time approach is adopted where transport is simulated through particle tracking. Local dispersion and diffusion are neglected; the dispersive behaviour depends on the spatially variable velocity field only. An effective aperture (porosity) in the model is calibrated such that predicted and measured travel times coincide. The results of the numerical flow and transport models are verified against an analytical solution for a homogeneous case.

The complete listing of prediction results are presented in Ström (1996, 1997); in the present report the used methodology and results are discussed in more detail. Results are analyzed in terms of the output entities (drawdown, breakthrough curve, travel times, recovery) and performance measures (accuracy measure, uncertainty measure) defined in Ström (1996). The results indicate that the conditioning specifically reduces the uncertainty in drawdown. It is shown to be important to include steady-state head values during pumping in order to reduce uncertainty in predicted drawdowns. The conditioning also reduces uncertainty in transport related entities such as travel time; however, the reduction is smaller. Finally, the conditioning results in transmissivity fields with a more pronounced spatial structure.

The prediction of the radially converging experiment was in general more successful than the dipole predictions. This is mainly due to the fact that a calibrated aperture was obtained from a preliminary tracer test previously conducted; only the pumping rate was different between the preliminary test and the test to be predicted. However, in the radially converging experiment recovery was predicted from all four boreholes whereas

in the field test only recoveries from two borehole injections were obtained. The simulated results are sensitive to the not well-known head boundary conditions. The rough discretization, which is not fine enough to capture the details of the velocity field, is believed to be problematic specifically for the dipole predictions.

Finally, the sensitivity of the generated fields on assumed model parameters is investigated. Only the radially converging case is considered for transport in these comparisons. It is shown that the results are fairly stable with respect to changed parameters. A decrease in the correlation length results in fields with more variability. If the head boundary conditions are allowed to fluctuate, the variability of the fields are reduced. The resulting flow and transport entities generally follow the pattern of increase or decrease in transmissivity variability.

Appendix 3 Questionnair

APPENDIX 3 COMPILATION OF ANSWERS TO QUESTIONNAIRE CONCERNING TASK 4C AND 4D

QUESTION	CRIEPI	PNC/GOLDER	SKB KTH-CE	POSIVA	BMBF	SKB (KTH-TRUE)
1 Scope and Issues						
a What is your purpose of participation in Task 4?	Understanding of solute migration on detailed scale in crystalline rock. Usefulness of flow and transport models.	Improve understanding of flow and transport in 50m scale discrete fracture networks. Focus on transport and connectivity.	To increase our knowledge about flow and transport in fractured rock and also to apply CHAN3D to a specific experiment to test its capabilities and weaknesses. Furthermore, the simulations may be a help to illustrate the effects of different transport mechanisms.	To learn more about water flow and tracer transport in a heterogeneous single fracture as a basis for performance assessment. Carefully conducted tracer tests expected to reveal essential features of flow and transport processes.	Check knowledge of flow and transport mechanisms in fractured rock. Exchange experiences with international partners.	Part of TRUE team; predictions in Task 4 part of scopings, predictions and evaluation within TRUE. Overall objectives given by TRUE.
b What issues did you wish to address through participation in Task 4?	Description of heterogeneous geological feature with simple model.	Role of head field in modelling. Effect of intersecting fractures on transport. Difference between DFN, continuum and analytical solutions. Test of DFN models.	More knowledge on the important entities for fluid flow and solute transport such as flow distribution and void volume of the features.	Flow heterogeneity (channeling), flow rate distribution in fracture plane. Interaction rate transported solutes-fracture walls in various parts of the fracture.	Influence of heterogeneity of a fracture system on the flow system, understand transport of solutes in geosphere.	The possibility to decrease uncertainty and increase understanding in flow and transport predictions by using conditioning on available hydraulic data and comparing with experimental results.
2 Conceptual model and data base						
a To what extent have you used the data sets delivered? Task 4C: Data Distribution 1 and 4 plus the extra data set. Task 4D: Data distrib. 1&2.	Task 4C: Data delivery 1, 3, 5 Task 4D: Data delivery 1-2	The full Task 4C&D data sets where used for the DFN-model	Model for the RC test calibrated on data from preliminary tracer test. The breakthrough curves and drawdown from the RC test used to refine the boundary conditions and calibrate the model for the DP test	Only used interpreted data and data directly related to the modelled tracer tests. No raw data, eg pressure build-up test data.	Geological structure from 4A, hydraulic measurements and experimental data from preliminary tracer test and radially converging tracer test.	Task 4C: Data distribution 1,2, and 3. Task 4D: Data distribution 5 (task 4C) and 1.
b Specify more exactly what data in the data sets you actually used?	Geometry of Feature A. Geometry of boreholes. Transmissivity of sections. Injection and pumping rates. Drawdowns. Prior hydraulic head. Injection concentrations. Sampling flow rates. Breakthrough concentrations.	Packer tests, flow logs, interference tests to interpret hydraulic properties. Preliminary tracer experiments for transport properties for Task 4C. Results of 4C for transport proprieties for 4D. Geological information for DFN-model. Head data and dilution of injected tracers for BC and hydraulic properties of feature.	To define geometric model, locations of the "A" and "B", the tunnel, niche and boreholes were used. Transmissivity of "A" and "B", hydraulic conductivity of the rock mass and hydraulic head in the features were used, especially specific values for "A".	Task 4C: Injection and breakthrough curves drawdown from preliminary test. Hydraulic heads in natural flow field. Estimated lognormal T field of "A". Correlation length of T-field in "A". Task 4D: Updated measurements of hydraulic head in natural flow field.	Measurement of natural hydraulic head, preliminary tracer tests incl drawdown, tracer input data. Task 4D all delivered data used.	Task 4C: Transmissivity statistics and geometrical data of boreholes. Interference test data for conditioning and transport data for calibration, tracer injection concentration and pumping rate data. Task 4D: updated head values for renewed transmissivity conditioning. Breakthrough data from transport calibration (4C) and tracer injection concentration and pumping rate data.
c 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?	None.	Generic relationship between transmissivity and transport aperture. Fracture size distributions from adjacent drifts.	The hydraulic head at the boundaries in rock mass was estimated by using scarce data. The heads at the rock around the tunnel at the boundary plane that intersects the tunnel (south border of the model) were assumed.	Diffusivity of tracer in water. Assumption that isotropic lognormal T-field with spherical correlation can be applied.	None.	No additional data used.

QUESTION	CRIEPI	PNC/GOLDER	SKB KTH-CE	POSIVA	BMBF	SKB (KTH-TRUE)
3 Model geometry and structural model						
a How did you geometrically represent the TRUE-1 site and its features/zones?	Feature A modelled as single flat square with side 30 m	Analytical solutions and continuum models treated "A" as single homogeneous plane. DFN model contained deterministic features (A, NNW, NW) and stochastic background features.	"A" was represented by a fracture plane extended to the boundaries. The fractures included in "B" represented by limited planes.	Only the "A" was modelled as a planar 2-D heterogeneous fracture.	Deterministic system with "A" and "B" as planar "D features based on the structural model from Winberg et al (1996) and cores and hydraulic tests.	Assumption of singular 2D feature (confined aquifer model)
b Which features were considered the most significant for the understanding of flow and transport in the TRUE- 1 site, and why?	Possible connections between "A" and other features	Background head field and intersecting discrete features.	"A" is the most important because most of the flow and transport occur in that feature. The intersection of the "A" with some plane of the "B" may explain the low recovery in RC for one of the cases.	Influence of all other features intersecting "A" were incorporated as background head field.	Weak connection between "A" and "B" which may be neglected.	The effect of the tunnel likely very important for gradient, which in turn determined transport characteristics.
4 Material properties						
a How did you represent the material properties in the hydraulic units used to represent the TRUE-1 site?	Spatial distribution of transmissivities in "A" by kriging based on drawdown from tracer experiments	Most models treat discrete features as homogeneous and isotropic planar aquifers. Sensitivity studies with stochastic transmissivity fields for "A"	The rock mass and "A" and "B" are represented by a network of channels conductance distribution. For "A" and "B" were mean values derived from T of these features. The mean value for the channel conductance in rock mass was calculated from the rock mass K. SD is taken from measurements at the Äspö site.	"A" modelled as heterogeneous fracture with lognormal T-field and spherical correlation length. Additional fitted coefficient for ratio between hydraulic and transport apertures of fractures.	Hydraulic conductivity, fracture aperture and special storage coefficient are important to represent the hydraulic behaviours in the fracture system. Water saturation state from TRUE-1 experimental site. Hydraulic conductivity and fracture aperture were varied in order to describe the hydraulic flow field reasonably.	Spatially variable transmissivity with assumed distribution and correlation structure (stochastic continuum approach).
b What is the basis for your assumptions regarding material properties?	T in "A" show lognormal distribution and correlation in spatial distribution	Fracture T based on: TRUE Team report, analysis of dilution history, calibration of drawdown. Transport apertures based on Doe Law with calibration to previous tracer tests.	The assumptions are based on geometrical considerations and observations that fluid flow and solute transport occur through channels in fractured media.	Lognormal T-field applied generally based on experiments from many studies. Separate transport and hydraulic apertures needed because of numerical difficulties in solving head field with large variance in T.	Zero special storativity assumed if the gas saturation in the pore and water compressibility could be neglected when the hydraulic pressure magnitude in the experiments didn't differ from the natural condition.	Hydraulic-structural investigations may be interpreted such that "A" is singular well-connected feature and less-connected with the surrounding.
c Which assumptions were the most significant, and why?	Spatial correlation of T since it is a prerequisite for kriging	Head field assumptions and definition of DFN for understanding recovery and dispersion. Intersecting background fractures for drawdown.	The most important assumptions are the properties of the features A and B, as most of the water flows through these features.	For breakthrough times and drawdown that the ratio hydraulic/transport aperture is fixed single number fitted with preliminary tracer test data. Parameter only valid for that test configuration.	In the homogenous model the fracture aperture was often considered as a constant, which is a most significant factor that influences the distribution of flow field and thereby the transport velocity of tracer.	Assumption of singular feature most significant, if wrong the approach is questionable and obtained understanding may be misleading.

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5 Boundary conditions						
a What boundary conditions were used in the modelling of the TRUE-1 tests?	Fixed hydraulic head on boundaries. No flux of tracer across boundaries. Time-varying tracer flux at injection boreholes.	Combination of fixed heads at boundaries and time-varying flux in pumping wells.	Constant hydraulic head on the vertical sides, top and bottom. In the model, one boundary plane intersected the tunnel set at hydraulic head of tunnel. Pumping and injection flow rates used when applicable. Assumed that the conductivity of fractures is reduced a factor of 10 near the tunnel surface.	Fixed hydraulic head boundary condition by linear extrapolation of measured fresh water heads in natural flow conditions.	The piezometric head on all boundaries of "A". Specified flow rate was used in the injection and pumping situation.	Specified head along all four boundaries.
b What was the basis for your assumptions regarding boundary conditions?	Head at distance point unaffected by pumping and determined by fracture zones and tunnel. "A" does not intersect with other fractures, thus tracer migration only in "A".	Heads, tracer dilution and flux rates from data distributions.	In the rock, the pressure is almost constant, decreasing slightly in the tunnel direction. The most of the pressure difference is found around the tunnel	Assumed that "A" is large fracture with intersections to other hydraulic active fractures far from test area.	Calculation area twice the experimental site to ensure that the boundary condition on the outer boundary is unaffected by the experiments.	Simple head isolines drawn from undisturbed head in boreholes. Originally heads from regional model planned to be used, the adapted methodology chosen since head in boreholes also were used in conditioning.
c Which assumptions were the most significant, and why?	No change in head on boundaries during tests. Natural gradient influences recovery.	Background head field controlled direction of transport and recovery.	The extent of the "A". If assumed that "A" reaches model borders, reasonable drawdown obtained. If "A" is limited, not reaching borders, unrealistic drawdowns are obtained.	Extrapolated fixed head boundary condition not valid if intersections with well conducting fractures are close to pumping hole.	Correct pumping rate in the experimental boreholes important because it determines the flow configuration of the experiments.	Boundary conditions of "A" in undisturbed state also applied for pumping period.
6 Model calibration						
a To what extent did you calibrate your model on the provided hydraulic information? (steady state and transient hydraulic head etc.)	Spatial distribution of transmissivities in "A" estimated to minimise sum of squared normalised errors in drawdown. Natural gradient from observed heads in boreholes during steady state.	Boundary conditions conditioned to match in situ heads in "A". Transmissivity derived from dilution measurements.	Boundary conditions and transmissivity of the features A and B were estimated from the hydraulic information (steady state)	Drawdown from preliminary tracer test to calibrate ratio between hydraulic and transport apertures.	Calibrated flow model with a steady hydraulic head under the natural flow condition and the condition of the preliminary tracer test in the 4C and additionally under the condition of RC-1 in the 4D.	Conditional simulations made with measured transmissivity and steady-state head (prior and during pumping) to obtain T-field. Denoted conditioning since well defined parameters were used.
b To what extent did you calibrate your model on the provided "transport data"? (breakthrough curves etc.)	Fracture aperture and longitudinal dispersion estimated to minimise difference between calculated and measured breakthrough.	Transport aperture based on generic relationship. Dispersion values derived from breakthrough curves.	Void volume of the "A" used in RC-1 was determined from the preliminary tracer tests. For the dipole tracer test, the void volume of "A" was refined by using the breakthrough curves from RC-1.	Breakthrough from preliminary tests used to calibrate ratio between hydraulic and transport apertures.	Based on the flow field calibrated by hydraulic head, the breakthrough curve from PTT and RC-1 (breakthrough time, maximal concentration and tailing form of the curve) have been calibrated in the transport model.	Evaluated mean travel times from previous experiments to calibrate transport porosity. Denoted calibration since transport porosity serves as fitting parameter.
c What parameters did you vary?	Transmissivities except KA3005A R3. Natural hydraulic gradient. Fracture aperture. Longitudinal dispersivity.	Head boundary conditions. Transport aperture.	Skin factor limiting the water flow into the tunnel varied in some simulations. Small skin factor gives large fraction of injected tracer into tunnel. Transmissivity of "A" varied to match drawdown in injection and extraction sections.	Variance of lognormal T-field varied during calibration.	Local distribution of the hydraulic conductivity. Fracture aperture. Flow porosity. Dispersivity and diffusion	Transmissivity statistics and transport apertures.

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d Which parameters were the most significant, and why?	Fracture aperture most significant.	Transport aperture - breakthrough times. Mass recovery - head filed and connectivity.	Impact of certain parameters different in flow model compared to transport model. Transmissivity of "A" significantly influences the flow model (drawdown), but influence on transport model negligible as flow in feature is given. Boundary conditions influence fluid flow and solute transport in a significant way.	Variance in T-field and ratio between hydraulic and transport apertures seems coupled. To explain drawdown and transport time larger variance of T-field needed than possible for numerical reasons.	Flow geometry and hydraulic conductivity were the most significant - determined the tracer transport path and time	Expected value of trans-missivity most important to predict drawdown. Transport porosity most important to predict breakthrough. Too low transmissivities underestimates drawdown, Since no mass transfer breakthrough determined by injection function and porosity alone.
e Compare the calibrated model parameters with the initial base, comments	Large difference in T for estimated value and data base for KXTT3 R2. Drawdowns there cannot be explained by initial data.	Key model parameters: Background head field (changed during experiment), feature transmissivity (changed by reconfiguring packers), Transport apertures (calibrated different from initial), Dispersion lengths (adjusted from initial)	In general, no large differences are found between the model used in the prediction of the RC tests and the model used for prediction of the DP tests. No conditioning of the trans-missivity at the injection or extraction locations were performed.	Calibration indicated larger variance of T-field than estimated in structural model. Understandable since estimate in structural model based only on hydraulic information.	NONE GIVEN	Expected value and variance of transmissivity higher than initial values. For heterogeneous simulations is fitted porosity lower than initial. For homogeneous porosity coincide.
7 Sensitivity analysis						
Identify the sensitivity in your model output to: **a) The discretisation used**	Not sensitive to discretisation due to small elements near borehole.	No studies made. For the present model and unconditioned Stochastic Continuum affects primarily effective dispersion parameters. May be replaced with homogeneous model and scaling.	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.	Resulting dispersion depends to some extent on discretization.	Two different meshes were used to identify the sensitivity of the discretisation of the finite element	Two case considered: 1 $\Delta x=\Delta y=0.4$m and $\Delta x=\Delta y=0.2$m. For hydraulics refinement not very important. For transport refinement gave better resolution.
b) The transmissivity (distribution) used	Drawdown very sensitive to spatial distribution of transmissivities in "A". Breakthrough also sensitive to distribution in T, but less because of fixed pumping rate.	Magnitude of drawdown directly related to spatial pattern and magnitude of T.	The mean value of the transmissivity distribution was varied in order to match the drawdown in the injection and extraction sections. The transport of the tracer is almost no influenced by variation in the transmissivity of the "A", since the flow rate into the extraction section is given.	Mean transmissivity may have strong influence on recovery. Applied correlation length not so important.	The hydraulic conductivity and fracture aperture have been varied.	See Model calibration above.
c Sensitivity to transport parameters	Breakthrough sensitive to aperture and longitudinal dispersivity.	Breakthrough times to aperture and dispersion scales with longitudinal dispersivity.	Transport parameters. The flow porosity or the volume of the channels is directly correlated with the residence time.	Fitted ratio hydraulic/transport aperture controls breakthrough time.	Additionally transport para-meters, e.g. flow porosity, dispersivity and diffusion coefficient were checked in order to determine their influences on the transport phenomena.	See Model calibration above.

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8 Lessons learned						
Given your experience in implementing and modelling the TRUE- 1 site, what changes do you recommend with regards to: **a1 to experimental site characterisation**	Confirming whether "A" intersects with other fractures or not.	More instructive to use all information (heads, interference data, flow logging, BTHV) rather than ignoring to build simplified model. More accurate characterisation of head field and connectivity structure before tracer tests. Extended interference testing with interpretation. How can a simple confined aquifer model be used given the interference responses and flow dimensions. Recommend more evaluation of results to improve conceptual model. Conceptual model consistent with data as far as possible, and should guide iterative process of testing.	If the aim is the prediction of tracer tests on the detail scale, the experimental site characterisation is good enough.	More thorough flow rate (dilution) measurements in both natural conditions and forced conditions.	The experimental site of TRUE was very good characterised.	Better understanding of boundary conditions needed.
a2 Recommended changes to experimental design	Reverse test of DP-1 and DP-5,6	Pumping rates as low as possible for better understanding of local head fields and heterogeneities. Scoping calculations to set time scales, pumping rates, mass recovery. TRUE-1 experiments point out difficulties in tracer tests in less transmissive features, changing flow fields, multiple intersecting fractures, significant heterogeneity.		Shorter, better defined and measured source terms.		Important to have good knowledge of the injected mass flux (the flux only obtained by estimating flow rate from injection concentration curve through fitting). This results in a subjective (somewhat uncertain) input flux.
a3 Recommended changes to presentation of characterisation data		Low mass recovery more educational than high mass recovery, although no mass recovery raises more questions than answers.	The presentation of character-isation data is not good. The characterisation data are mixed with conceptual models and other simulations.	Emphasis on transient behaviour of transport (following the decay of the source term tailing is of no interest).		No comments.
a4 Recommended changes to performance measures and presentation formats	Linear instead of logarithmic graphs for breakthrough curves.	Mass recovery, mean break-through time are fundamental measures. Useful to give dispersion (t5 & t95) normalised to t50 rather than as absolute numbers, due to linear scaling with aperture. Mass recovery used for understanding existence of multiple pathways. Mass recoveries were given for specified time, which confuses with transport time. Projected ultimate mass recovery is an additional performance measure.	Regarding performance measures and presentation formats they are not adequate. Due to the short travel times of the experiments and the slow decay of the injection curve, the times to recover 5, 50 or 95% has almost the same meaning. A very important entity in tracer tests, the travel time, was omitted in Task 4C. It was, however, included in Task 4D.	Performance measures based on long lasting injection curves are irrelevant, e.g. t50 or t95 of the whole injection curve.		Very hard to come up with good and general measures. There has been a lot of discussion on measures in conjunction to presentation of results, but very little input on the measures prior to predictions.

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b What additional site specific data would be required to make a more reliable prediction of the tracer experiments?	Spatial distribution of "A"	More detailed analysis of performed interference tests helpful in defining structural/ hydraulic connectivity model for "A". Additional analysis of transient hydraulic responses in injection/pumping intervals for understanding of transmissivity structure near wells. Transport aperture patterns and relationships between transmissivity, storativity, transport aperture and fracture roughness.	Better knowledge of the boundary conditions, head at different locations at the rock mass	Flow rate distributions in the fracture also in various scales, e.g. in boreholes intersecting the fracture close to each other (20-50 cm)	The additional measurement of the concentration in the other boreholes and / or in the interval of Feature B will give us more detail information about tracer distribution in the fracture system.	Data base is good enough. However, still a lack of understanding of the processes.
c What conclusions can be made regarding your conceptual model utilised for the exercise?.	Experimental results of RC-1 and DP 1-4 can be reproduced by using simple model of "A"	Models used by the AMTF in general too simple to properly represent flow and transport in "A". DFN approach generally used for stochastic predictions from statistical data. Tasks 4CD shows DFN can be conditioned for useful representations of specific hydraulic structures. For assumptions and parameter values see draft reports.	See tables below.	The conceptual model explains the dispersion behaviour reasonably well.	Feature A could be considered as a planar fracture system regarding our conceptual model. But the channelling effect may exist and it could be described as one dimensional element in a two dimensional model.	Feature A is not a singular feature unconnected to its environment, but for prediction of drawdown in boreholes the model is quite adequate.
d What additional generic research results are required to improve the ability to carry out predictive modelling of transport experiments on the detailed scale?	Research for the relation between dispersivity and spatial distribution of fracture aperture.	Generic information concerning the nature of flow and transport at fracture intersections, the effects of mineralizations and infillings, and the generic relationship among transmissivity, storativity, transport aperture and roughness would be helpful.	Research to obtain information about the flow wetted surface, and how this entity is correlated with the water flow rate.	The flow field has to be solved (theoretically or experimentally) in the scale of cm:s in the transport path region before any sensible transport predictions can be made.	On the detailed scale one can use another geoscientific method, e.g. radar tomograph to detect the distribution of tracer concentration during the tracer test so that it could be as additional information for the modeller.	A need to understand the relation between hydraulic and transport apertures in order to make blind predictions of transport (i.e. Without site-specific data from tracer tests).

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9 Resolutions of issues and uncertainties						
a I What inferences did you make regarding the descriptive structural hydraulic model on the block and detailed scale for the TRUE- 1 site?	We inferred that "A" was highly heterogeneous in regard to transmissivity. Transmissivities in vicinity of KXTT3 R2 are estimated to be very high.	"A" is at least a heterogeneous fracture and more likely a set of intersecting discrete fractures. The pressure responses and transport pathways between boreholes probably occur in fracture net-works rather than a single intersecting fracture. Low drawdown indicates that intersecting features makes "A" to behave as a leaky aquifer. The 50m scale DFN at TRUE-1 site provides time-varying global boundary conditions for transport.	CHAN3D resolves fluid and solute transport in channels or fractures. It includes addiction in the channels and interaction with the rock matrix. For sorbing tracers, sorption in matrix is included. The model has been tested for different scales. From several 100s m in LPT2, down to a few 10s m in these predictions. In task 4C&D, the detail scale, only advection and dispersion by channelling were active, since interaction with the rock matrix is negligible due to the short contact time.	It is reasonable to model "A" as a hydraulically rather isolated 2-D object.	In the fracture system Feature A, which was quite well-known, the tracer tests were interpreted by numerical model. The consistency of the geological model and the numerical model were proved.	See question: Material properties, Basis for assumptions.
b What issues did your model application resolve?	The issue of how we express a heterogeneous geological feature by a simple model consistently with experimental results.	Model addressed the need to include intersecting discrete features even when modelling a relatively simple, small scale discrete fracture.	See above	Mean transport aperture (which was already calibrated) and some dispersion behaviour.	The tracer transport parameter (effective porosity, dispersivity and diffusion coefficient) were determined by the modelling of the tracer tests under different test configurations. The num-erical models Rockflow (flow model and transport model) applicability have been tested.	The reduction in prediction uncertainty by use of head and transmissivity data resolved. The model works well for predicting drawdown.
c What additional issues were raised by the model application?	The relation between dispersivity and spatial distribution of fracture aperture.	4C: Importance of addressing global boundary conditions. 4D: the complexity of pressure response, mass recovery and breakthrough curves in "A" perhaps corresponding to the existence of a network of features within "A".	No other issues	Comparing modelling results with experiments cannot uni-quely distinguish between various concepts and model-ling assumptions. Iterative cycles of experiments and modelling is required to test critically model performance.	The question is if the model and parameter can be used in a large scale consideration. The extrapolation of the result from detailed scale to large (real) scale should be investigated in the next step.	See Lessons learned, Additional generic research needed.

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