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Overall evaluation of the modelling of the TRUE-1 tracer tests – Task 4

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

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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. The task was carried out in 1995–2000 and consisted of several modelling exercises in support of the TRUE-1 tracer tests, including predictive modelling where experimental results were not available beforehand.

This report presents an overall evaluation of the achievements of Task 4. The specific objectives of the overall evaluation were to highlight innovative and successful modelling approaches developed, to assess the stages of the task which proved most beneficial for conceptual understanding of transport processes at the TRUE-1 site and to assess the success of various steering tools.

A concise summary of scientific achievements is given and conclusions drawn with respect to unresolved technical issues. Recommendations are presented that can optimise the management of future modelling tasks.

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1 Introduction

1.1 Background and scope

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 the behaviour and properties of the natural geological barrier, investigate interactions between engineered barriers and the host rock and develop and demonstrate technology for deep repository systems.

Within the Äspö Hard Rock Laboratory project, a programme called Tracer Retention Understanding Experiments (TRUE) has been defined for performing tracer tests on different experimental scales. The overall objectives are to increase the understanding of the processes that govern retention of radionuclides in crystalline rock and to increase 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 on different scales and with successively increasing complexity.

The first stage (TRUE-1) was completed in 2000 (TR-00-07). Tracer tests with both non-sorbing and sorbing tracers were performed on a detailed scale (<10m) with the objective of studying flow heterogeneity, transport connectivity and sorption processes and evaluating relevant transport parameters. Further objectives were to test and improve methodologies for tracer injection and sampling and the use of weakly and moderately sorbing tracers. Additional experiments performed within TRUE-1 concern analysis of fracture aperture distributions by resin injection in fractures and testing sampling and analysis technologies for evaluating matrix diffusion. The work performed within TRUE-1 was, to a large extent, a learning exercise, contributing data and experience for the more elaborate tracer tests performed within the TRUE project, e.g. the TRUE Block Scale Project.

The Äspö Task Force on Modelling of Groundwater Flow and Transport of Solutes was set up by SKB in 1992 as a forum for international cooperation in the Äspö Hard Rock Laboratory. The work of the group is performed on well defined and focused modelling tasks in the area of conceptual understanding and mathematical modelling of groundwater flow and solute transport. The Task Force selects specific experiments to be performed in the Äspö Hard Rock Laboratory (HRL) for parallel modelling by the Task Force organisations. Each organisation supporting the Äspö HRL is invited to form or appoint a team to carry out modelling of the experiments. The modelling efforts of the Task Force provide information on how different model concepts can be applied in fractured rock and, in particular, allow identification of important parameters needed to perform predictive modelling of radionuclide transport.

Modelling Task 4 was carried out in 1995–2000 and consisted of several modelling exercises in support of the TRUE-1 tracer tests, including predictive modelling where experimental results were not available beforehand. The participating organisations and modelling teams are shown in Table 1-1. Task 4A consisted of modelling in support of development of a 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 aimed at predictive modelling of non-sorbing tracer tests at the TRUE-1 site, including a comparison of model outputs with experimental results. All these tasks were to a great extent, preparatory steps for Tasks 4E and 4F that comprised predictive modelling of tracer tests performed with a range of sorbing, slightly sorbing and non-sorbing tracers.

Table 1-1. Organisations and modelling teams participating in Task 4.

Organisation	Modelling team	Modelling Task					
		4A	4B	4C	4D	4E	4F
ANDRA	CEA-DMT			X		X	X
BMWi (BMBF)	BGR			X	X	X	X
CRIEPI	CRIEPI			X	X	X	X
DOE	LBNL	X					
DOE	SANDIA						X
JNC (PNC)	Golder Associates	X	X	X	X	X	X
NAGRA	PSI					X	X
POSIVA	VTT Energy		X	X	X	X	X
SKB	KTH-ChE			X	X	X	X
SKB	KTH-TRUE	X	X	X	X	X	X
UK Nirex	AEA Technology		X	X			

1.2 Objectives

Modelling Task 4 consisted of a total of six subtasks with multiple objectives such as experimental design, predictive modelling, tracer test analysis and development of conceptual transport models. The history behind the Task is also complex – the subtask definitions were often driven by urgent needs of the TRUE-1 field programme.

Given the complexity of Task 4 and its long duration of more than 5 years, the Task Force Delegates felt a strong need to perform an overall evaluation of the achievements of the Task. The expectations of the Task Force focused not only on a compilation of the scientific output but also on assessing the evolution of conceptual understanding and various aspects of task management. The specific objectives of the overall evaluation were defined as follows:

- to highlight innovative and successful modelling approaches developed in the course of Task 4,
- to assess those stages in the evolution of the Task which turned out to be most beneficial for conceptual understanding of transport processes at the TRUE site,
- to assess the success of various steering tools (definition of performance criteria, blind predictions, questionnaires, etc).

Finally, a concise summary of scientific achievements is given and conclusions drawn with respect to unresolved technical issues. Recommendations are presented, aimed at optimisation of task management for future modelling tasks.

1.3 Expectations of the participating organisations

Participation of the organisations in Task 4 of the Äspö Task Force was motivated by a common interest in basic research in the field of modelling flow and transport processes in fractured hard rock. Beyond this, each organisation gave emphasis to specific aspects of relevance to their national waste disposal programmes. The specific expectations were then summarised by the Task Force Delegates of each participating organisation and include:

- a brief outline of the motivation for participation (e.g. international cooperation, education of modelling groups, etc),
- a reference to the topical focus (site characterisation, performance assessment, etc),
- a link to the national program (waste type, host rock formations, etc).

ANDRA

Initially and within the framework international cooperation, the participation of ANDRA in Task 4 had two main goals: i) gaining experience in single fracture characterisation in fractured granite and ii) validating modelling tools and methodologies. The major output of this project is a conceptual understanding of transport processes resulting from the predictive modelling of the tracer tests (particularly the sorbing tracers). The interaction of the flowing tracers with the surrounding materials leads to a better understanding of diffusion and surface sorption processes and parameters which are necessary for estimating the performance of the geological barrier.

The ANDRA/CEA modelling group participated in Tasks 4C (Predictive modelling of radially converging tests), 4E (Scoping calculations on sorbing tracer tests STT-1) and 4F (Predictions for sorbing tracer tests STT-2), and used the CASTEM 2000 numerical code developed at CEA.

Today, in addition to the Clay Project Division, which is in charge of clay URL construction in eastern France, the new Granite Project Division is seeking knowledge that could be acquired from an operational granite URL abroad in order to complete a 2006 document prior to the siting process for a URL in granite. The results of Task 4 will contribute to the siting procedure in terms of understanding flow and transport processes in fractured hard rock.

BMWi

BMWi is funding non site-specific applied basic research into underground disposal of radioactive waste. The research programme comprises issues related to the host rock formations rock salt, argillaceous material and crystalline rock. The majority of the research activities are carried out in international projects. Investigations into geological disposal in crystalline rock are carried out at the Grimsel Test Site and at the Äspö HRL.

One of the main objectives of these activities is to support research aimed at broadening and consolidating the understanding of groundwater flow and radionuclide transport in fractured rock. The DURST/ROCKFLOW numerical programme was developed to simulate these processes. The programme is being continuously refined. The TRUE-1 experiments provide a series of well documented experiments which are very well suited for validation of the numerical models in a water-saturated rock environment by comparing calculation results and results of in situ experiments carried out under realistic conditions. In addition, the Task Force provides an opportunity to cooperate with highly motivated experts from those countries and groups that are conducting research in this field.

CRIEPI

In October 2000, the Nuclear Waste Management Organization of Japan (NUMO) was established with responsibility for implementing geological disposal of high-level radioactive waste. By 2005, NUMO will select potential candidate sites on the basis of the results of area-specific literature surveys. Next they will perform geophysical explorations and geological surveys using boreholes at the sites and will select candidate sites by 2008. Finally, through detailed site investigations which will start in 2010 using boreholes and an underground investigation facility, they will select the disposal site by 2023. NUMO is considering crystalline rock as one of the candidate host rocks for the disposal facility. CRIEPI has the role of providing technical support for NUMO’s activities. CRIEPI has therefore developed numerical analysis codes to predict groundwater flow and solute migration in fractured rocks accurately. CRIEPI has obtained data on the hydraulic conductivity and migration characteristics of the fractures and the rock matrix of granite rocks through laboratory experiments, since it is very difficult to perform any in situ tracer experiments using radionuclides in Japan at present. The purpose of CRIEPI's participation in Task 4 is to deepen understanding of migration phenomena of sorbing solutes in fractured rock through numerical analyses of the in situ tracer experiments and to assess the usefulness of its developed numerical codes, FEGM and FERM, for the prediction of such phenomena.

DOE/Sandia

Sandia National Laboratories (SNL) has the role of science advisor to the U.S. Department of Energy (DOE) with respect to the WIPP transuranic waste repository. A critical component of the performance assessment calculations done by SNL for the WIPP site is the potential transport of radionuclides through a fractured dolomite. In order to achieve a better understanding of the role of dual-porosity transport in this dolomite, a series of non-sorbing tracer tests was conducted at the WIPP site in 1995 and 1996. The results of these tests and subsequent laboratory analyses showed the influence of multiple rates of diffusion. A multi-rate numerical model was constructed and successfully used to interpret these tracer tests.

Motivation for SNL and the DOE to participate in the Äspö Task Force is driven mainly by the desire to apply the multirate model to tracer tests conducted in a fractured rock environment different from that at the WIPP site. The TRUE-1 tests provide a documented set of well executed experiments. These test results are well suited for further verification of the multirate model in a different fractured rock environment. Additionally, sorbing tracer tests were not conducted at the WIPP site and participation in the Äspö Task Force allows SNL and the DOE to test the Multi-rate model on sorbing tracer test results.

In addition to testing numerical and conceptual models of solute transport developed at the WIPP site, participation in the Äspö Task Force allows for cooperation with the nuclear waste programs of multiple countries. These interactions have proven to be beneficial to SNL and the DOE in better understanding solute transport in fractured rocks.

JNC

The Nuclear Waste Management Organization of Japan (NUMO) has been established to implement geological disposal of HLW in Japan and JNC's role is to conduct basic research to enhance confidence in geological disposal. JNC is now carrying out in-situ experiments at the Mizunami Underground Research Facility for crystalline rock and the Horonobe Underground research facility for Tertiary sedimentary rock. However, both URLs are still at the surface investigation stage and JNC would like to gain experience from Äspö before starting the operational stage in Japan. One of the findings of the H12 PA report which was published by JNC in 1999 was that retardation between canister and the nearest major water-conducting feature is most important for the retardation in the geosphere. Also, JNC believes that the retardation process operating in the crystalline rock is generic, although some parameters are different. Äspö provides a unique opportunity to study transport processes in crystalline rock in detail. JNC is interested in understanding transport processes and the site characterization method, used to derive relevant parameters.

NAGRA

Modelling of radionuclide transport in the context of Nagra's R&D programme has been an important research issue for more than 15 years. The radionuclide migration experiment (MI) at the Grimsel Test Site formed the experimental framework and the modelling group of the Paul Scherrer Institute (PSI) provided the scientific resources. Key objectives of the numerical studies were model and code development, model calibration, upscaling of sorption coefficients and predictive modelling. The applicability of relatively simple dual-porosity models was demonstrated successfully for predictions of radionuclide transport in the MI shear zone on a scale in the meter to decameter range.

The hydrogeological and hydrochemical conditions at the Grimsel Test Site (e.g. low fracturisation, microstuctural features of fractures, low mineralisation) are far from being representative for the crystalline basement in Northern Switzerland, which is a candidate host rock formation in Nagra's high level waste programme. Participation of the PSI modelling group in Task 4 was therefore motivated by the wish to assess the applicability of their modelling approaches in a different environment. Special focus was given to development of microstructural conceptual models of flow porosity, based on geological analysis of the water-conducting features at the TRUE-1 site. In addition, upscaling approaches were tested using sorption data from the supporting laboratory studies. Validation of PSI's modelling approach was carried out in the framework of Tasks 4 E and F.

Beyond the aforementioned specific issues, as part of its international collaboration programme it is in Nagra's general interest to benefit from scientific interaction with other groups of highly motivated modellers. Know-how in the field of transport modelling is expanded and deepened and scientific credibility increased by active participation in international research groups.

Posiva

Posiva participated in Task 4 to assess the concept for groundwater flow and transport of solutes used when evaluating the performance of the geosphere as one of the sequential barriers that retard and disperse potential releases from a repository. The coupling between flow and the extent of interaction of solutes with surrounding solid materials, such as surface sorption and matrix diffusion, has been of special interest.

Possibilities to study different concepts of streamtube geometry and material around and within the streamtube are one aspect of Posiva's motivation. Tracer tests performed in-situ also offer the possibility to test the idea of determining the flow-related part of transport at a site and material properties regarding retardation in a laboratory. Experiments performed in a well characterised single feature, as in Task 4, provide a basis for analyses of more complicated flow and transport systems.

SKB

Basic research for understanding the processes of transport and retention was carried out in the Stripa mine as a joint project within the OECD/NEA cooperative framework. It was considered necessary to perform such experiments also in a rock which had not been subject to the hydraulic drawdown that for a long time had prevailed at the Stripa mine. This was also the case for chemically related research and together these constituted a strong reason for establishing the Äspö Hard Rock Laboratory.

The purpose of the TRUE-1 experiments from the SKB standpoint is to gain an understanding of flow and solute retention processes in a generic sense, such that these results can be “calibrated” with the site specific conditions of the repository candidate sites investigated by SKB. The results obtained from the TRUE-1 experiments and the work within Äspö Modelling Task Force are expected to provide valuable input to the next real site performance assessment, which is planned to start in the next few years.

2 Task 4 – Overview

This chapter contains an overview of Task 4 of the Äspö Modelling Task Force, including the purpose and scope of the task, a brief presentation of the Task Force modelling groups and the task history. Since Task 4 consisted of modelling exercises in support of the TRUE-1 tracer tests performed at the Äspö Hard Rock Laboratory the chapter starts with a brief summary of the relevant parts of the TRUE-1 project.

2.1 Overview of the TRUE-1 experiment

The objectives of the first stage (TRUE-1) were to conceptualise and parameterise an experimental site using both conservative and sorbing tracers in a simple test geometry on a small scale. The experiments were primarily aimed at technology development and constituted a platform for the subsequent experiments within TRUE. The scope of TRUE-1 included characterisation of the site, developing the experimental methodology and performing and evaluating the experiments.

2.1.1 TRUE-1 site characterisation

The 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 metres. A detailed characterisation programme has been performed at the site, including five cored boreholes (KA3005A and KXTT1–KXTT4). The characterisation included analysis of pressure responses 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, cross-hole interference tests, hydrogeochemistry, preliminary tracer tests and tracer dilution tests.

2.1.2 Structural model of the TRUE-1 site

Based on the resulting database, a structural model was built (ICR 96-04), see Figure 2-1. Three minor fracture zones (NNW-4, NW-2 and NW-3) were identified and interpreted as boundaries of the TRUE-1 block. In addition, a structurally less well defined zone (NW-2') was identified.

Four minor features (Features A, B, C and D) were identified in the borehole array. Feature A is a steeply dipping, NW trending structure characterised as a reactivated mylonitic structure. Features B and D are structurally more complex, consisting of a number of different planar fractures with a wide spread in orientations forming NW – trending features intersecting Feature A south of the borehole array. Feature C is interpreted as a single gently dipping fracture (not shown in Figure 2-1).

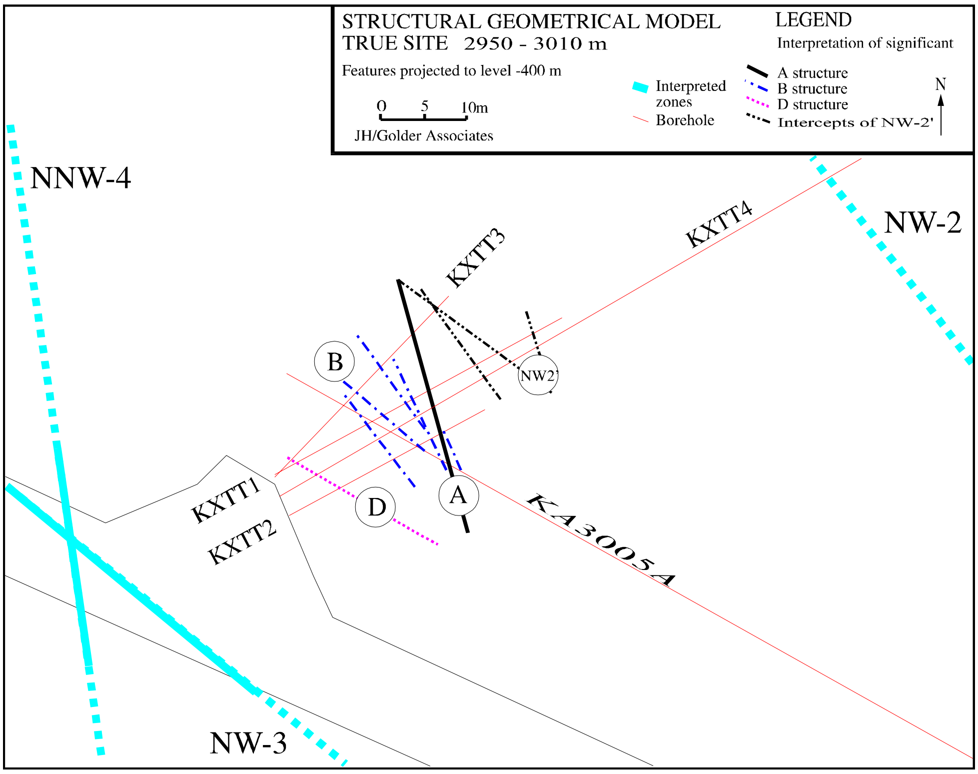


Figure 2-1. *Structural and geometric model of the TRUE site. Horizontal section at Z=–400 m showing bounding minor fracture zones and features identified in the TRUE-1 block (from ICR 96-04).*

Feature A essentially follows the mylonite, but is partly in contact with altered Äspö diorite. Results of the tracer tests show that the feature is connected over the entire area covered by the borehole array. There are indications from tracer tests and detailed flow logs and the BIPS (Borehole Image Processing System) that several flow paths exist within Feature A. Pressure response during pumping tests also indicates that Feature A is divided into fractures (splays) towards the tunnel.

2.1.3 Update of the TRUE-1 structural model

An update of the structural model of the TRUE-1 block was presented to the modellers before the predictions of STT-2 (Task 4F). The description of the updated model was also documented in the TRUE-1 Final Report (TR-00-07). The update contained a more detailed description of Feature A. The updated model included the initial characterisation data (cross-hole interference tests, hydraulic head data, hydraulic tests, initial tracer tests), the outcome of work performed as a part of the Fracture Classification and Characterisation project (FCC) and the results of the tracer test programme (RC-1-RC-3, DP-1-DP-6, STT-1, STT-1b, STT-2).

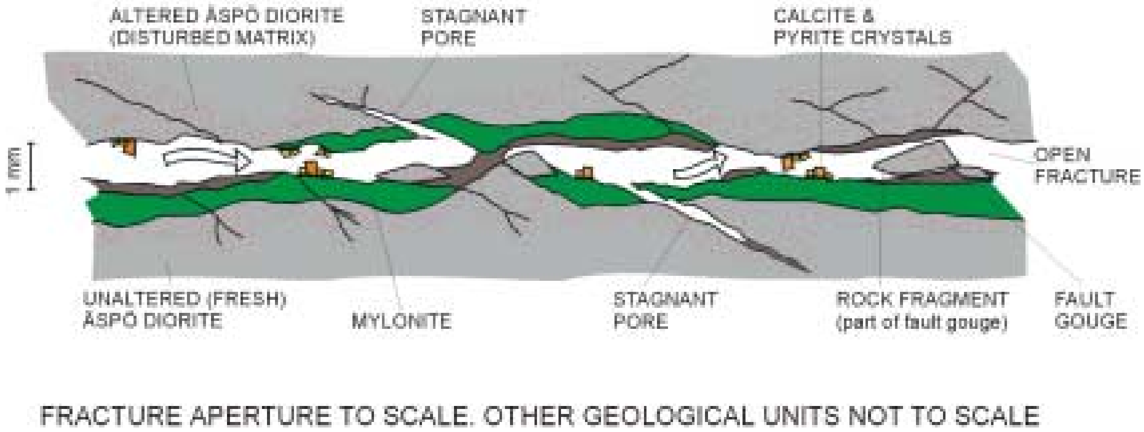


Figure 2-2. *Schematic conceptual representation of Feature A (from TR-00-07).*

The update confirms the major findings of the initial characterisation work (ICR 96-04), but emphasises the presence of splays giving more than one intercept of Feature A in several of the boreholes. The update also included a refinement of parameters for Discrete Fracture Network (DFN) modelling based on the FCC work. Furthermore, additional results were presented from laboratory experiments providing data for transport parameters.

Figure 2-2 shows the schematic conceptual representation of Feature A presented by the TRUE-1 project (TR-00-07). The feature essentially follows the mylonite, but can in part be in contact with altered Äspö diorite. Scanning electron microscopy and energy dispersive spectrometer (SEM/EDS) analysis showed the presence of clay minerals as an outer rim of the fracture mineral coating. This was taken as an indication that gouge material may be present in Feature A. Fault gouge material has been found in similar features at Äspö, but has not been isolated in the cored boreholes performed in Feature A.

2.1.4 TRUE-1 tracer experiments

A large number of tracer tests have been performed in the borehole array penetrating Feature A. Selections of these tests have been included in the Task 4 predictive modelling work. Figure 2-3 shows the test geometry and the interaction pattern with Feature A of the radially converging test RC-1 (Task 4C), the dipole test DP1–DP4 (Task 4D) and the sorbing tracer tests STT-1 and STT-1b (Task 4E) and the sorbing tracer test STT-2 (Task 4F).

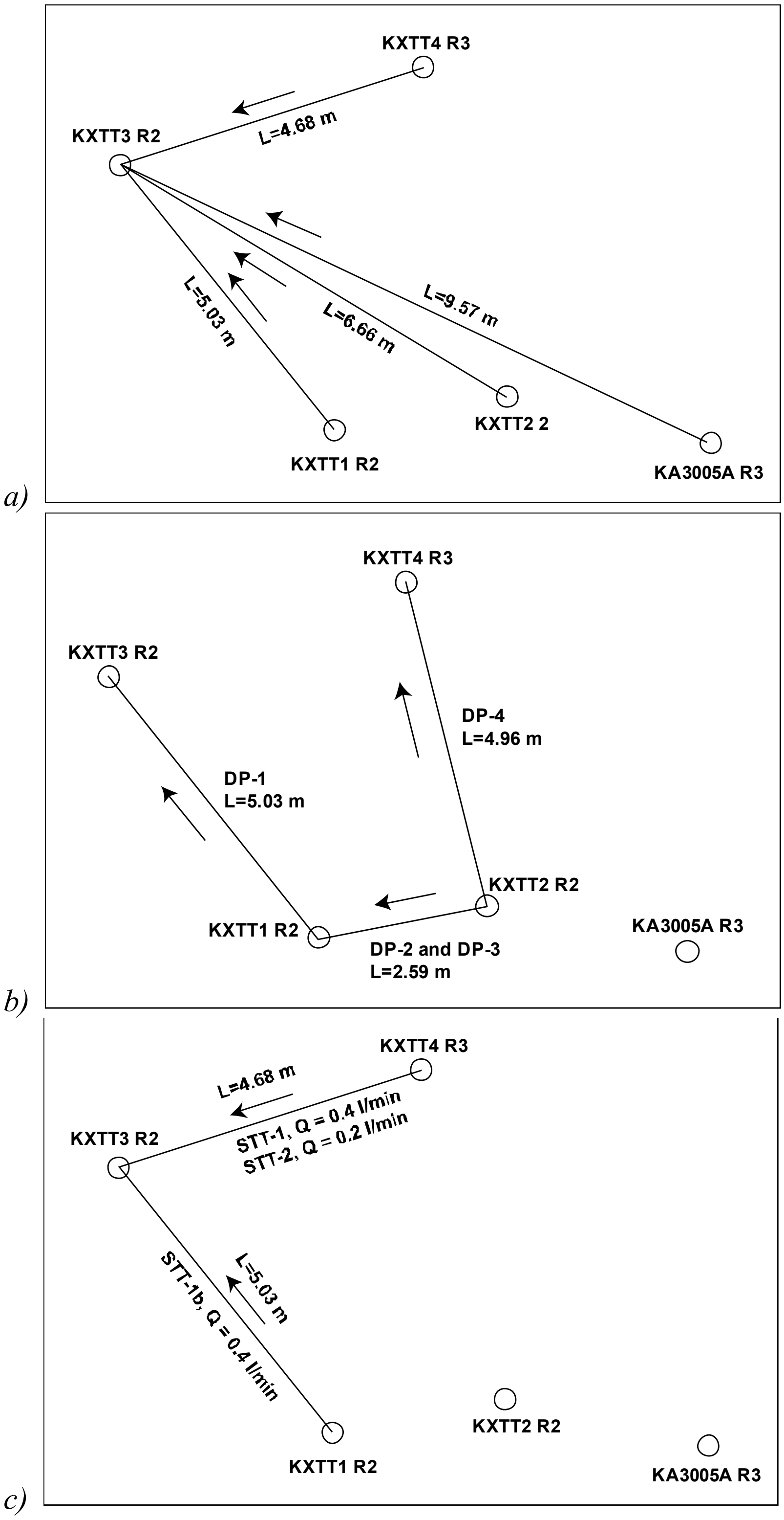


Figure 2-3. *Test geometry, pumping flow rates (Q) and borehole intersection pattern with Feature A for a) the TRUE-1 Radially converging tracer test (RC-1), b) the Dipole test (DP1–DP4), c) the sorbing tracer tests STT-1, STT-1b and STT-2.*

2.1.5 TRUE-1 continuation project

After the finalisation of the first TRUE stage, additional tests with the existing installations were performed to explore some unresolved issues from the previous tests (IPR 02-47). The purpose was to obtain more information on the connectivity between Feature A and the surrounding fracture network, and to explore the internal structure of Feature A, in particular the reason for the double peak observed in the breakthrough from the STT-2 test.

Five different test set-ups were made, the first three (CX-1 to CX-3) comprised tracer dilution tests combined with pumping and the last two (CX-4 and CX-5) consisted of multiple hole tracer tests.

In the pressure interference tests CX-1 and CX-2, pumping was performed in borehole sections intersecting Feature A, KXTT4 and KXTT3, respectively. The response in sections which included Feature A was fast and significant, while sections including the bounding fracture zone NW-2 showed a fast, but significantly smaller response. Sections including Features B and D responded slower with less response. The interference test CX-2 with pumping in a borehole section of KXTT4 intersecting Feature B gave a fast significant response in borehole sections interpreted as being associated with Features B and D, while the response was significantly smaller in sections which included Feature A. Very limited response was obtained in the bounding fracture zone NW-2.

The tracer test CX-4 was performed to investigate the reason for the double peak observed in the STT-2 test. The injection section in KXTT4 was divided into two sections, each including one of the intersections believed to belong to Feature A. The test was performed in a radially converging flow-field similar to that used in STT-2, i.e. pumping in KXTT3:R2 at a rate of 0.2 l/min, but with injection of different tracers in the two injection sections. The test indicates the presence of two individual flow paths, with distinctly different mean travel time and dispersivity. However, in comparison with the STT-2 test, it was noted that the travel time was considerably longer, although the same pumping rate was used. The reason for the slower transport is not clear, but it may be caused by altered hydraulic characteristics and a changed flow pattern.

The tracer test CX-5 was aimed at assessing the connectivity between Feature B and Feature A. Pumping was made in KXTT3 in Feature A at a rate of 2.97 l/min. Tracer was injected in two sections intersecting Feature A and two sections intersecting Feature B. Breakthrough was detected only from the injection points in Feature A, while no breakthrough was detected from the injection points in Feature B over a period of 700 hours.

The interpretation of the complementary investigations at the TRUE-1 site was that they generally confirmed the existing hydrostructural model (ICR 96-04), i.e. the TRUE-1 test array consists of at least three well separated hydraulic units, Feature A, Feature B+D and Feature NW-2. The investigators conclude that the flow regime may not be considered as three-dimensional on the scale of the tracer tests performed within TRUE-1. However, on a larger scale the features are interconnected.

2.2 Task concept

The purpose, scope and working methods of the Äspö Task Force are defined in the Task Force Charter. The purpose is to provide a forum for interaction in the area of conceptual and numerical modelling associated with the experimental work performed at the Äspö HRL. The work is focused on conceptual understanding rather than producing scientific data. The way to achieve this is to set up well defined and focused modelling tasks. Typically, several modelling teams address each task using a wide spectrum of approaches. The modelling teams are provided with background information and data concerning the site and the set-up of the experiment, but are allowed a large degree of freedom in approaching the modelling task.

The steering tools used by the Task Force are primarily the periodic meetings (1–2 per year). The Task Force meetings included presentations of results, technical sessions where the modelling teams had the possibility to review and evaluate the work and executive sessions for discussion and decision on the evolution of the task. Minutes of the discussions were taken and, since the 10th Task Force meeting proceedings were prepared containing a compilation of results and interim reports from the modelling groups. The meetings also provide opportunities for interaction between experimentalists and modellers. If required, modelling group meetings are held between the Task Force meetings.

The modelling teams were requested to provide modelling reports for the completed tasks. Questionnaires for the different tasks were prepared to collect information from the modelling groups on scope, conceptual and numerical models, data usage and lessons learned. To simplify the comparison of results, several types of performance measures were defined, providing measures of accuracy and uncertainty.

2.3 Aims and overview of subtasks within Task 4

Modelling Task 4 consists of several modelling exercises in support of the TRUE-1 tracer tests with the following objectives:

- to perform predictive modelling of tracer tests on a detailed scale using site characterisation data (understanding of flow and transport processes at the site),
- to propose configurations and procedures for tracer tests (experimental design),
- to assess the value of the available site characterisation data and the proposed configuration and procedures (optimisation of site characterisation procedures).

The predictive modelling was based on data on fracture geometry, rock and fracture mineralogy and petrology, transmissivity, storativity, fracture connectivity, matrix diffusivity and tracer sorption properties provided by the TRUE-1 site characterisation programme.

The Task Force considered it important for a large number of modelling groups to work on a selection of well defined modelling tasks. The TRUE-1 tracer experiment was seen as a unique opportunity for inter-comparison of modelling approaches.

Task 4 contained elements of structural modelling based on site characterisation data, tracer test design and planning, predictive modelling and process evaluation. It also involved a lot of interaction between the TRUE Project Team and the Task Force modelling groups. Therefore, the modelling tasks were defined in close relation to the scope of the TRUE Project Team. However, the work of the Task Force provided valuable complementary modelling approaches. Task 4 was divided into six separate subtasks with different scope and objectives. The scope and objectives of the different subtasks are outlined in Table 2-1.

Table 2-1. Scope and objectives of modelling subtasks in Task 4.

Task	Scope / Definition	Objective
4A	To perform modelling in support of a descriptive structural model of the site.	Assist TRUE Project Team in developing a structural site model.
4B	To perform modelling in support of experimental design.	Assist TRUE Project Team in designing tracer experiments.
4C	To perform predictive modelling of the radially converging tests in Feature A. Comparison of model output with experimental results.	Develop understanding of radionuclide migration and retention in fractured rock. Evaluate the usefulness and feasibility of different approaches to modelling radionuclide migration. Evaluate what can be achieved with the existing TRUE-1 data set in terms of transport predictions.
4D	To perform predictive modelling of the dipole tests in Feature A using RC-1 as calibration cases. Comparison of model output with experimental results.	Establish boundary conditions of Feature A. Evaluate what can be achieved with the existing TRUE-1 data set in terms of predictions for non-sorbing tracers.
4E	Performance of predictive modelling of the TRUE-1 tracer tests with sorbing tracers (STT-1 and STT-1b). Comparison of understanding of radionuclide migration and retention in fractured rock. Evaluation of what can be achieved with existing data from the TRUE-1 site in terms of predicting transport of solutes subject to sorption.	Develop understanding of radionuclide migration and retention in fractured rock. Evaluate the usefulness and feasibility of different approaches to modelling radionuclide migration of sorbing species based on existing in situ and laboratory data from the TRUE-1 site.
4F	Performance of predictive modelling of the TRUE-1 tracer tests with sorbing tracers STT2 with the updated structural model. Comparison of understanding of radionuclide migration and retention in fractured rock. Evaluation of what can be achieved with existing data from the TRUE-1 site in terms of predicting transport of solutes subject to sorption. Comparison between the predictions from the new structural model and the old experimental results.	Develop understanding of radionuclide migration and retention in fractured rock. Evaluate the usefulness and feasibility of different approaches to modelling radionuclide migration of sorbing species based on existing in situ and laboratory data from the TRUE-1 site.

2.4 Modelling groups and approaches applied

A total of eight modelling teams representing seven organisations performed predictive modelling of the TRUE-1 tracer tests in Tasks 4C and 4D. Different modelling approaches and models were used, see Table 2-2. 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 were used with different approaches for assigning the properties of the fracture. For the heterogeneous models both deterministic and stochastic representations were used. To a varying degree, fractures connected to Feature A have been considered in the models, for example through the use of discrete fracture network models and channel network models.

Nine modelling teams, representing eight organisations, performed predictive modelling in Tasks 4E and 4F, applying a wide range of models and modelling approaches, see Table 2-3. The main focus of the work was on the transport of sorbing tracers, while the flow modelling generally received less attention than in the previous tasks. The modelling groups basically retained the model geometry and structural model used in the predictions of the non-sorbing tracer experiments in Tasks 4C and 4D. However, the need to include relatively complex transport processes in the models led in many cases to a need to simplify the geometric description of Feature A.

Table 2-2. Approaches applied by modelling groups for Tasks 4C and 4D.

	CRIEPI	**PNC/Golder**	**SKB KTH-ChE**	**POSIVA/VTT**	**BMWI/BGR**	**SKB KTH-TRUE**	**Andra**	**Nirex/AEA**
FLOW MODELLING								
Type of model	Deterministic continuum model (Stochastic in predictive modelling)	a)Deterministic continuum model b)Discrete fracture network model (DFN)	Channel network model	Stochastic continuum model	Deterministic continuum model	Stochastic continuum model	Analytical model	Stochastic continuum model
Process description	Water flow in heterogeneous 2D fracture.	a)Water flow in a homogeneous 2D fracture. b)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 a heterogeneous 2D fracture	Water flow in 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 an infinite plane	Feature A modelled as a heterogeneous plane, 25x20 m
TRANSPORT MODELLING								
Type of model	Deterministic continuum model	Deterministic continuum model Discrete fracture network model (DFN) Analytical model	Channel network model	Stochastic continuum model	Deterministic continuum model	Stochastic continuum model	Linear stochastic model	Stochastic continuum model
Process description	Advection, longitudinal and transverse dispersion.	Advection Longitudinal and transverse dispersion Advection, dispersion Advection-dispersion in radially converging homogeneous flow field in dual porosity medium.	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, longitudinal dispersion	Advection, spreading due to Taylor dispersion
Geometric framework and parameters	Feature A modelled as single flat square with side lengths 30m.	a)Feature A modelled as single flat square with side lengths 48 m. b) 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 c) Feature A modelled as infinite flat square	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.

Table 2-3. Approaches applied by modelling groups for Tasks 4E and 4F.

	CRIEPI	**JNC/Golder**	**SKB KTH-ChE**	**POSIVA/VTT 4E**	**BMWi/BGR**	**SKB KTH-TRUE**	**Andra/CEA**	**Nagra/PSI**	**DOE/Sandia**
FLOW MODELLING									
Type of model	Deterministic continuum model	Discrete fracture network model (DFN)	Stochastic, Discrete Channel Network	4E) Stochastic continuum model 4F) Analytical channel model	Deterministic continuum model	Stochastic continuum model	Analytical and stochastic continuum models	Deterministic continuum model.	Water velocity estimated from non-sorbing tracer breakthrough
Process description	Water flow in heterogeneous 2D fracture and homogeneous 3D rock matrix.	Water flow in discrete 3D fracture network.	Water flow in a heterogeneous 3D channel network	4E) Water flow in heterogeneous 2D fracture. 4F)Water flow through rectangular parallel plate channel	Water flow in heterogeneous 2D fracture	Water flow in a 2D planar fracture with spatially variable aperture.	Water flow in a homogeneous/ heterogeneous 2D fracture	Water flow in a 2D homogeneous fracture.	
Geometric framework and parameters	Feature A heterogeneous fracture plane, 30x30 m Rock matrix on each side of Feature A modelled as 3D homogeneous block, 30x30x0.1 m	Modelling of feature A (RC) and zone NW-2* + a highly conductive pathway between KXTT2-KXTT3 (DP) + stochastic background fractures in a 50 m rock block.	Tunnel with niche, Feature A and B. Feature A is extended to the boundaries and Feature B is confined. The size of the modelled rock volume was 30 x 30 x 40m.	4E) Feature A modelled as heterogeneous fracture plane,15x11 m 4F) Activated flow path(s) represented as single or several parallel flow channels	Feature A modelled as heterogeneous fracture plane, 20x20 m. Feature B included but with negligible influence	Feature A is modelled as a 20×20 m planar fracture with spatially variable aperture.	Feature A modelled as a 2D plane. Radial flow field approximated as uniform.	Feature A is modelled as a planar fracture.	
TRANSPORT MODELLING									
Type of model	Deterministic continuum model	Deterministic continuum model	Stochastic, Discrete Channel Network. Particle tracking	4E) Particle tracking Analytical 4F) Analytical channel model	Deterministic continuum model	Lagrangian stochastic advection reaction	Linear stochastic model	Deterministic continuum model.	Multirate mass transfer model
Process description	Feature A: Advection, dispersion, surface sorption Rock matrix: Advection, dispersion, diffusion and sorption	Advection-dispersion, surface sorption, matrix diffusion and sorption	Advection and matrix diffusion-sorption, spreading due to transport in different channels. Sorption in fracture filling material	4E) Advection, Dispersion due to spatially variable velocity and random component in particle tracking. Surface sorption Matrix diffusion and sorption 4F) Advection, molecular diffusion in the advective flow field, diffusion into fault gouge or stagnant zones, diffusion into rock matrix	Advection, longitudinal and transverse dispersion, diffusion, and sorption in fracture plane, sorption into the matrix	Advection-dispersion due to velocity variation, Diffusion/sorption into rock matrix, Diffusion into stagnant water, Sorption on fracture surface and gouge material	Advection, dispersion Surface sorption Matrix diffusion and sorption	1D-advection, (longitudinal) dispersion, linear sorption, limited 1D-matrix-diffusion. Optional: spatially variable velocities.	Advection dispersion Mass-transfer by diffusion and sorption
Geometric framework and parameters	Feature A as heterogeneous fracture plane, 30x30 m Rock matrix on each side of Feature A modelled as 3D homogeneous block, 30x30x0.1 m	1 to 9 pathways derived from DFN modelling.	Transport in Channels and diffusion perpendicular to the fracture plane.	4E) Transport in 1D flow paths derived from flow modelling. Unlimited matrix. 4F) Activated flow path(s) represented as single or several parallel flow channels	Feature A modelled as heterogeneous fracture plane, 20x20 m. Feature B included but with negligible influence	Flow path with unlimited matrix.	1D flow path with limited matrix	Feature A modelled as a network of two (independent) fracture families.	1D flow path with mass transfer to layered blocks

2.5 Task history

A schematic description of the Task 4 chronology is given in Figure 2-4. The programme shows the extension of the TRUE tracer experiments, the Task 4 subtasks and interaction in the form of data deliveries to the modelling teams. Furthermore, the dates of the Task Force meetings are indicated.

The proposal for modelling Task 4 of the Äspö Task Force was presented at the 5th Task Force Meeting in Kuhmo, Finland (November 29 to December 1 1994) with the title "Predictive modelling of non-sorbing tracer tests on a detailed scale during the first TRUE stage". At the time, the TRUE-1 experiment had not yet started. The objectives of the proposed task were:

- to perform predictive modelling of non-reactive (conservative) transport on a detailed scale using site characterisation data,
- to propose configurations and procedures for tracer tests with conservative tracers,
- to define what information regarding solute transport can be determined given available site characterisation data and the proposed configuration and procedures.

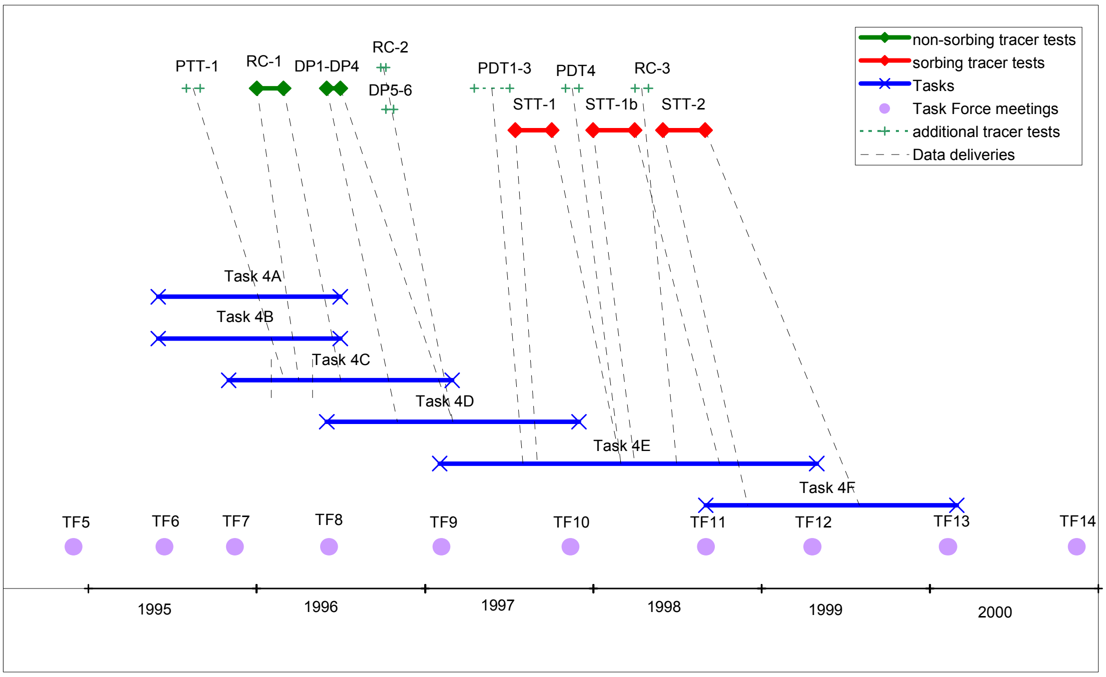


Figure 2-4. *Chronology of Task 4 and link to TRUE-1 project plan.*

Task 4 was further discussed at the 6th Task Force meeting in Västervik, Sweden in June 1995 and at two preceding Task working meetings. Drilling had now been performed at the site and four features of potential interest had been identified. The geological structure of the site was discussed and it was concluded that a good structural model was needed as a basis for the predictive modelling. At the Task Force meeting it was decided that the TRUE project team should produce a data package for Task 4, including the raw data from the site characterisation. The TRUE team was also to interpret the data and establish a structural model of the site. This data package was to provide information for the modelling groups that wished to set up alternative structural models. The Task Force could in this way assist the TRUE Project Team in the site characterisation work. The need for preparatory modelling work to evaluate uncertainties and tracer test configurations was also identified.

Task 4 was redefined based on the discussions at the 6th Task Force meeting and the three subtasks 4A, 4B and 4C were defined. The input (data packages) and expected output of the different subtasks were defined. Task 4A and to some extent also Task 4B were performed in close interaction between the TRUE Project Team and the Task Force modellers. A draft version of the modelling in support of development of a structural model (Task 4A) was presented at the 7th Task Force meeting in Hergiswil, Switzerland in November 1995. At this time, the site characterisation programme had identified Feature A as the most promising structure as it appeared to be structurally and hydrogeologically more simple than the other features. Preliminary tracer tests had been performed, indicating a good hydraulic connectivity but shorter travel times than expected. Scoping calculations of the TRUE-1 experiment had also been performed (Task 4B). These indicated that a single flow path could be expected for the radially converging tracer test and that matrix diffusion would not be important for the chosen tracers on the short timescale of the experiment. Task 4C was further defined and the objectives developed. The radially converging tracer test with tracer injection at four locations (RC-1) was chosen for the predictive modelling. Performance measures were proposed, including measurements of drawdown, breakthrough curves, predictions of breakthrough at certain times and predictions of mass recovery. For the stochastic models, statistical measures of the ensemble results should be given.

A total of eight modelling groups performed predictive modelling of the radially converging tests in Task 4C and the results were presented and discussed at the 8th Task Force meeting in Hultsfred, Sweden in June 1996. Topics that were brought up in the discussion included the possibility to derive relevant transport parameters considering the short timescale of the experiment and the long tail in the injection curve. The long injection pulse used in the tracer test was considered unsuitable for modelling. Several suggestions were put forward on how to design the ongoing and forthcoming dipole tests in order to increase the amount of information obtained concerning boundary conditions and flow heterogeneity.

The predictive modelling of the dipole test was defined as Task 4D and the results from seven modelling groups were presented at the 9th Task Force meeting in February 1997 in Cherbourg, France. The importance of a proper evaluation of the modelling task was recognised, including clarification of assumptions made by the modelling teams, analysis of reasons for differences among predictions and detailed studies of breakthrough curves. The usefulness of predictions based on pulse input function was also identified.

A proposal for Task 4E was also presented at the 9th Task Force meeting, comprising predictive modelling of the TRUE sorbing tracer tests performed during the summer of 1997. The tests were initially planned to be performed in the same flow path using three different pumping rates. A combination of non-sorbing, weakly sorbing and moderately sorbing tracers were to be used. The task was divided into a prediction phase and an evaluation phase.

The preliminary design tests performed in the summer of 1997 (PDT-1–PDT-3) indicated that tracer tests with the lowest pumping rates would not give the desired recovery and instead two tracer tests should be performed with the highest flow rate (400 ml/min), with injection in KXTT4 (STT-1) and in KXTT1 (STT-1b).

A total of eight modelling groups performed predictions for first part of Task 4E (STT-1). The predictions, together with the experimental results, were presented at the 10th Task Force meeting in Kamaishi, Japan in November 1997. The modelling teams continued to analyse and evaluate the results. The next step of Task 4E involved predictions for the STT-1b test with no updating of the structural model or calibration on experimental results from STT-1. Instead, the updated structural model was to be used for the evaluation part of the modelling task.

Predictions for STT-1b were presented at the 11th Task Force meeting in Äspö, Sweden in September 1998. In the discussions it was noted that the shape of the input curve affected the breakthrough curve and made it difficult to make a proper analysis. It was decided to perform a deconvolution of the experimental breakthrough curve in order to obtain a unit response curve. This curve could then be compared with modelling performed with pulse input functions. It was further decided to include prediction and evaluation of the STT-2 tracer experiment as Task 4F. The predictions of Task 4F should be based on the updated structural model.

Nine modelling groups presented predictions for Task 4F (STT-2) at the 12th Task Force meeting in Gimo, Sweden in April 1999. In the comparison between experimental data and modelled results, the overall impression was that most of the modelling teams had underestimated the arrival times for the sorbing tracers. The evaluation of the modelling of the previous tracer tests led to requests for complementary studies including further laboratory measurements of Kd and sorption. Also the need for resin injection and excavation of Feature A after finalising the tracer tests was emphasised. It was further decided that there should be an external evaluation of the modelling work performed within Tasks 4E and 4F and that there should be an overall evaluation of Task 4.

At the 13th Task Force meeting in Carlsbad, USA in February 2000, the modelling groups' evaluation of the Task 4E and 4F modelling was presented. The discussion that followed indicated that there are different views on the relative importance of flow and transport processes. The discrimination between heterogeneity and processes was discussed. The modelling indicates that the two peaks in the STT-2 breakthrough are due to geometry and not to tracer injection methodology. The results of the complementary laboratory measurements on diffusivity and sorption were presented.

Task 4 overall evaluation was initiated at the 14th Task Force meeting at Säröhus, Gothenburg, Sweden in November 2000. A brainstorming meeting was held where possible evaluation issues were listed, cf Chapter 3.1.

3 Evaluation issues

3.1 Areas of interest and evaluation approach

The motives of the organisations for participation in Task 4 were widespread – as stated in Chapter 1.3 the expectations included rather general aspects such as research and development in the framework of international cooperation, training of modelling groups as well as specific topics like benchmarking of numerical transport codes for performance assessment. This overall task evaluation is an attempt to assess the achievements and the unresolved issues from the viewpoint of the Task Force Delegates as representatives of their funding organisations. In addition, it should account for the overall mission of the Task Force, acting as an interface between site characterisation and performance assessment groups. Below are some of the key questions which formed the starting point for this evaluation:

- How did the level of conceptual understanding of solute transport at the TRUE-1 site change in the course of Task 4 and which were the most successful stages?
- Was there any valuable impact of Task 4 modelling results on the design of the TRUE-1 field experiments?
- Which site characterisation data improved conceptual understanding of flow and transport processes at the site?
- What conclusions can be drawn with respect to the suitability of the wide range of codes and model concepts?
- Which of the steering tools applied during Task 4 (questionnaires, blind predictions, performance measures, etc) are recommended for future modelling tasks?

Most of the questions are closely related to the long and complex history of Task 4 and its interaction with the TRUE-1 field programme (cf Chapter 2). The subtask definitions were often driven by the progress of the field programme, which made a rigorous analysis of achievements rather difficult. These preconditions – a wide spectrum of expectations of the Task Force Delegates and a complex task history – suggested restricting the focus of this task evaluation to a few nevertheless well defined topics.

Definition of the areas of interest was initiated during the 14th TF Meeting at Säröhus, Gothenburg. In a brainstorming meeting, the Task Force Delegates were asked to specify their wishes concerning the issues to be addressed in the overall evaluation task. The deliverable of the brainstorming meeting was a long list of items, reflecting a first, as yet unstructured scope of possible evaluation issues. A revised summary of the brainstorming meeting is given in Table 3-1.

Table 3-1. List of possible evaluation issues proposed by the members of the Task Force during a brainstorming meeting at Säröhus. This list formed the basis for the overall evaluation of Task 4 by the evaluation team.

- Methodologies for tracer test interpretation/analysis.
- Achievements in development of modelling tools.
- Evaluation of important Site Characterisation (SC) data.
- Role of modelling resources ("cost/benefit").
- Feedback by modellers to SC groups.
- Evolution of experimental and modelling ambitions.
- Evolution of the TRUE experiment.
- Most beneficial stages in the task evolution.
- Evolution of the conceptual model.
- Interaction between experimental and modelling groups.
- Aspects of steering a modelling task (interaction among modellers).
- Assessment of publication strategy.
- Relevance of flow model / microstructural models and processes.
- Evolution of SC focus / Optimisation of SC strategy.
- Transfer of evidence/parameters/methodologies to other sites ("effective properties"), robustness of statements.
- The role of modelling workshops / interaction between modellers.
- Transfer of understanding to other tasks (Task 5).
- Shortcomings of experimental set-ups (input pulse).
- Data deliveries (operation of interface SC/modellers/information overload).

Obviously, it was beyond the scope of this task evaluation to treat individually all the items that had been recorded in the brainstorming meeting. However, some of the issues could be grouped together, forming three main "areas of interest":

- assessment of conceptual understanding of transport processes with focus on Performance Assessment requirements (Chapter 3.2),
- achievements in tracer test interpretation (Chapter 3.3),
- assessment of steering tools as part of task management (Chapter 3.4).

Chapters 3.2 to 3.4 contain the statements of the actual evaluation issues for each of the areas of interest. The evaluation approaches are described and the achievements are assessed. Finally, a brief outlook is given, including recommendations for future modelling tasks.

3.2 Conceptual understanding of transport processes at the TRUE-1 site

3.2.1 Background and evaluation issues

The first tracer test cycle TRUE-1 constituted a training exercise not only for experimentalists but also for the modelling teams as part of the TRUE project and the Modelling Task Force, respectively. Among the experimentalists and modellers, the agreed strategy for improving understanding of reactive transport in fractured rock was to decompose the problem into two sub-problems:

- understanding groundwater flow in a complex hydrogeological environment,
- understanding transport mechanisms in a simplified flow pattern.

The concept of the TRUE-1 test cycle was to select a test site in a fairly well defined hydrogeological environment (single fracture with well defined boundary conditions and extensive hydrogeological characterisation of the site). It was expected that hydraulic characterisation of the site would lead to a satisfactory understanding of groundwater flow on the scale of the TRUE-1 tracer experiments. At this stage, a series of tracer tests with various flow geometries was planned, using non-reactive and reactive tracers.

The evolution of Task 4 was closely linked to the TRUE-1 concept. The early stages, Tasks 4A–D, were aimed at hydrogeological characterisation of the site (inventory of relevant structural features, estimation of hydraulic properties, definition of hydraulic boundary conditions); Tasks 4E and 4F were dedicated explicitly to the investigation of radionuclide transport and retention in fractured rock.

The following sections will highlight the achievements in understanding of groundwater flow (Chapter 3.2.2) and of transport mechanisms (Chapter 3.2.3) at the TRUE-1 site. The evaluation approach will address the following aspects:

- Which site characterisation (SC) data significantly improved the level of understanding? Conclusions will be drawn with respect to evaluation of SC data.
- Which interpretation steps / modelling tools provided particular insight into the problem? Focus is given to the power of model discrimination.
- To what extent did the different modelling approaches converge to a consistent conceptualisation of flow and transport processes at the site? How do parameter estimates compare to each other?

The evaluation approach requires a definition of the “level of understanding” as a basis for the assessment of achievements. We adopt a terminology consisting of three levels of understanding:

- **Plausibility:** The results of a conceptual/numerical model are plausible if they do not contradict general hydrogeological experience. This level of understanding does not allow any kind of model discrimination (“Which model is better?”).

- **Consistency:** If model results are consistent with independent evidence, confidence in general system understanding will increase.

- **Quantitative performance measures:** If the model output matches in a satisfactory way a quantitative performance measure, a certain amount of confidence in model predictions will result.

The final step in the evaluation approach includes a review of unresolved issues and a brief statement concerning transferability of the achievements to other sites.

3.2.2 Understanding of groundwater flow at the TRUE-1 site

Tasks 4A and 4B were aimed at assisting the TRUE Project Team to develop the structural site model (cf Table 2-1). The focus of Tasks 4C and 4D was on non-reactive transport in support of conceptualisation of groundwater flow at the site (boundary conditions of Feature A, hydraulic connectivity at the site). This early stage of Task 4 was strongly driven by the rapid evolution of the TRUE-1 project: final selection of the target Feature A, final design of the borehole arrangement and site instrumentation, frequent data deliveries with hydraulic test data and updates of the descriptive structural and hydraulic model. The challenge for the Task 4 modelling teams was to select their modelling tools and interpretation approaches with a rather premature understanding of the connectivity of the features, the heterogeneity of the site and the influence of the boundary conditions. This may be the reason that 6 of the 8 modelling groups chose a 2D representation of groundwater flow, which finally proved to be a major conceptual limitation.

Assessment of site characterisation data

A vast amount of site characterisation data (ICR 96-04, ICR 96-05; cf Table 3-2) was delivered by the TRUE-1 Project Team, including:

- various types of structural data (borehole logs, core logs, trace maps),

- mineralogical data (fracture mineralogy, SEM/EDS, thin-section analyses),

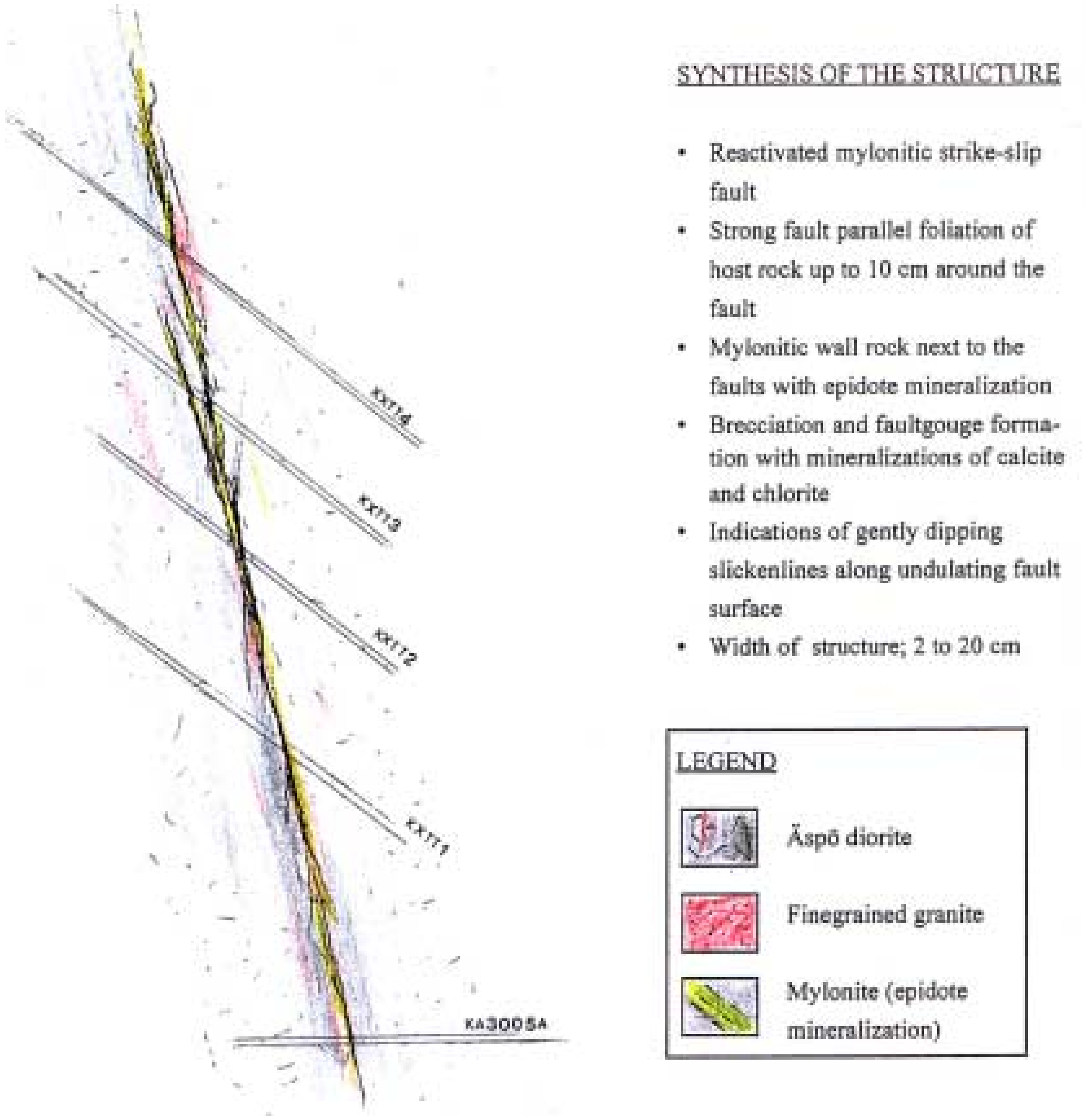
- hydraulic data (flow logging, dilution tests, packer tests, interference tests, long-term monitoring of hydraulic head),

- tracer test data (breakthrough curves of non-sorbing tracers).

Analysis of site characterisation data was carried out using a deterministic approach (cf ICR 96-04) and a discrete fracture network (DFN) approach with deterministic features and stochastic background fractures (cf ICR 96-05). Both approaches started by establishing an inventory of structural features at the site, using data from core mapping and tunnel mapping (for details cf ICR 96-04). Classification of structural features followed the general Äspö feature classification approach (TR-97-06).

For each borehole, a variety of indicative structural geological parameters (brittle deformation, large aperture, enhanced fracture frequency, etc) were used to assess the hydraulic relevance of the structural features. Hydrogeological assessment was complemented by the results of borehole flow logging and single-hole packer tests. Thus, structural and hydraulic attributes of the features were compiled along all boreholes. The next step was to correlate the features between the different boreholes. In the deterministic approach, this was accomplished in a rather qualitative way: features with similar attributes and consistent orientation were grouped together, finally forming a single hydraulic element on the scale of the TRUE-1 site. The stochastic approach made a more quantitative use of the SC data: statistics on fracture geometry (orientation, fracture frequency, trace length) were analysed, inflow locations and rates from flow logs were modelled and packer tests were simulated. The correlation of borehole intercepts together with pressure responses during drilling formed the basis for positioning the multipacker system for isolating the identified features. Cross-hole interference tests were performed to assess the connectivity of the isolated sections.

Finally, synthesis of structural and hydraulic data led to a conceptual description of the TRUE-1 site as given in Figure 2-1, consisting of 4 more or less planar features (Features A–D), each with a typical extent in the decameter range. Feature A was identified as the feature most relevant for the planned tests as it was judged to be structurally and hydrogeologically more simple than the other features. Figure 3-1 shows a conceptual structural model of Feature A as derived with the deterministic approach. Notably, no intersection of Feature A with Features B–D or NW-2 was implemented – Feature A is conceptualised as an isolated, more or less planar element. In Figure 3-2, a stochastic realisation of Feature A is given, consisting of three major elements: the deterministic features A and NW-2 and a stochastic system of background fractures.



SYNTHESIS OF THE STRUCTURE

- Reactivated mylonitic strike-slip fault
- Strong fault parallel foliation of host rock up to 10 cm around the fault
- Mylonitic wall rock next to the faults with epidote mineralization
- Brecciation and faultgouge formation with mineralizations of calcite and chlorite
- Indications of gently dipping slickenlines along undulating fault surface
- Width of structure; 2 to 20 cm

LEGEND

▨	Äspö diorite
🟥	Finegrained granite
🟩	Mylonite (epidote mineralization)

Figure 3-1. *Deterministic approach – Integrated detailed conceptual structural-geological model of Feature A, developed as part of Task 4A (cf Figure 5-4 / ICR 96-04).*

From a hydrogeological perspective, the structural descriptive models developed in the framework of Tasks 4A and 4B represent a plausible conceptualisation of hydrogeological conditions at the TRUE-1 site. The models are fairly consistent with the structural and hydraulic borehole data, but they do not represent the only possible conceptualisation. At this stage the information with respect to spatial continuity (in other words: hydraulic connectivity) of water-conducting features between the boreholes was limited.

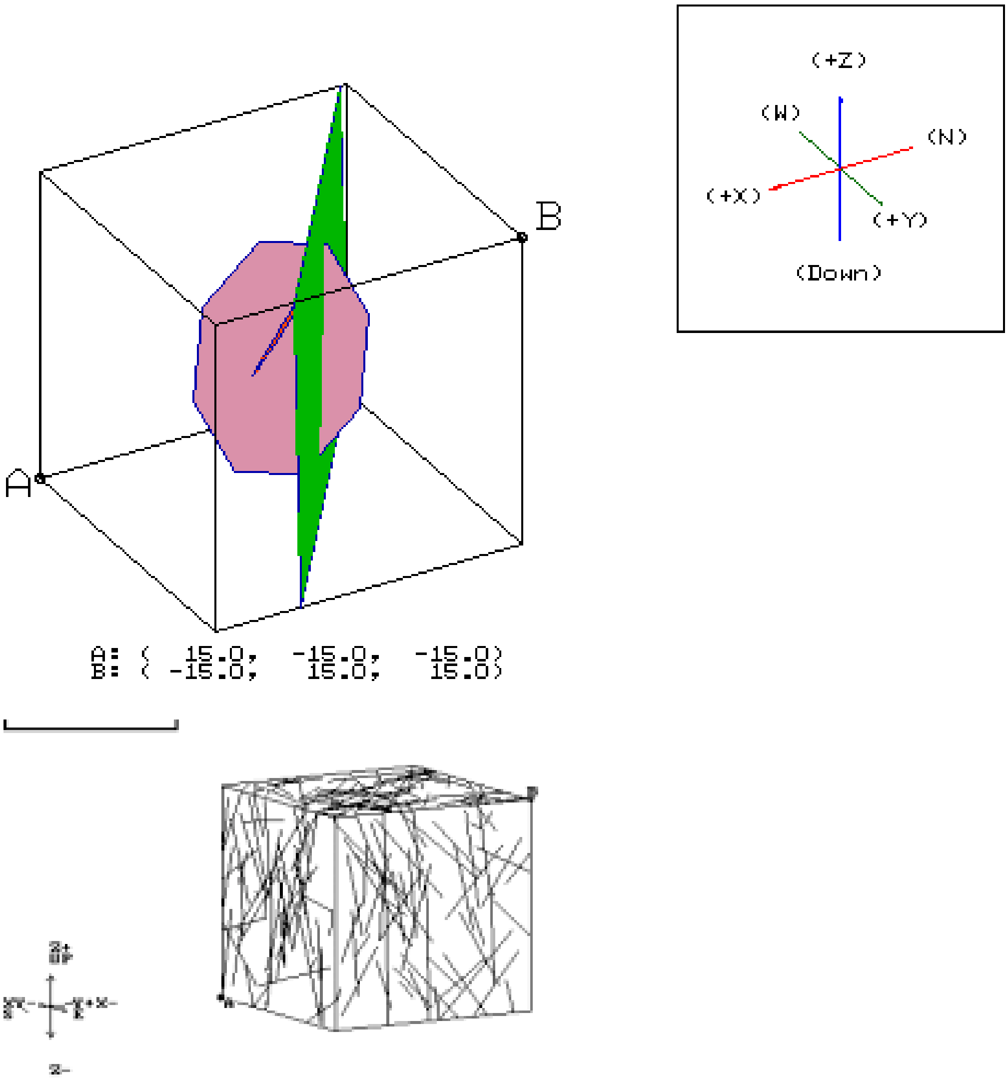


Figure 3-2. *Stochastic approach: deterministic Feature A, intersected by "NW-2" with a stochastic background fracture system (Figures 5-1 / 5-2 in ICR 96-05).*

The level of hydrogeological conceptualisation at the end of Task 4B formed the basis for the instrumentation of the TRUE-1 site. In particular, selection of packer locations and test interval lengths of the multi-packer systems relied on a suitable spatial definition of Feature A in all boreholes. A major risk of inappropriate instrumentation is the possibility of distortion of natural groundwater flow by short circuiting of the different water-conducting features through the boreholes.

When the site instrumentation had been completed, hydraulic interference tests, long-term monitoring of pressure and tracer tests were conducted to complement the site characterisation phase. These tests delivered extremely valuable data sets for validation of the structural descriptive model.

Analysis of interference tests indicated significant responses in borehole intervals, not identified with Feature A (cf ICR 96-05). Lack of reciprocity in test responses (i.e. comparison of normalised drawdowns, when source and monitoring wells are reversed) was interpreted as a response to complex boundary conditions and/or high spatial variability of hydraulic properties.

A rearrangement of the packer sections was made in December 1995 after the preliminary tracer test (PTT) and prior to the RC-1 test. The rearrangement was based on an evaluation of the hydrochemical data and generally consisted of a decreased length of sections connecting to Feature A and an increased length of sections connecting to Feature B. After reinstrumentation, the hydrochemical data within sections connecting to Feature A was much more consistent (TR-00-07).

However, the analysis of drawdowns during tracer test RC-1 showed clearly that the concept of a well separated Feature A does not hold and a leaky aquifer model was introduced to explain the hydraulic test responses.

Further inconsistencies were seen in the interpretation of long-term monitoring of pressure-build-up and of the RC-1 tracer test data. In fact, a revision of the hydrogeological model of the site at the end of Task 4D was not accomplished due to other priorities. It is believed that such a revision of the conceptual model would have considerably increased the insight into groundwater flow conditions at the TRUE-1 site.

Table 3-2 gives an overview of the available site characterisation data used by the different modelling groups. The relevance of these data for improving the understanding of hydrogeological conditions at the site is assessed in the last column. Summarising the experience during the early stages of Task 4, the following conclusions are drawn with respect to the site characterisation data:

- The conceptual descriptive model of the TRUE-1 site was largely derived from geological and hydraulic borehole data. Subdivision of the inventory of structural elements into 4 more or less independent planar “features” was plausible from a geological perspective, but was not the only possible interpretation.

- The instrumentation of the site was designed on the basis of the preliminary structural model where the spatial continuity of the features and possible interconnectedness was based on geological interpretations and pressure responses during the drilling. Based on the results of the initial hydraulic tests, a rearrangement of the packers was made prior to the tracer tests that were predicted within Task 4.

- Hydraulic interference tests and tracer tests proved to be suitable for evaluation of the conceptual model. However, the different interference tests could not be jointly interpreted with a single model, indicating an incomplete understanding of the hydraulic interconnectedness of the structural features at the site.

- Interference tests could have been used for refinement of the conceptual descriptive model. Due to its inherent flexibility, the stochastic modelling approach seems to be most promising for model refinement.

Possible revision of the conceptual descriptive model could have an impact on the instrumentation of the site, in particular leading to an optimised separation of the water conducting features. In conclusion, it is believed that incomplete understanding of the groundwater flow conditions at the TRUE-1 site is a major source of uncertainty in understanding of solute transport processes.

A number of unresolved questions concerning the connectivity between Feature A and the surrounding features, and the internal structure of Feature A were addressed by the complementary investigations performed within the TRUE-1 site, see Chapter 2.1.5. However, these investigations were performed after the finalisation of the modelling and evaluation work carried out within Task 4.

Table 3-2. Site characterisation data used in the course of TRUE-1.

Method	Purpose	Data used by:	Relevance[1]
Early stage of TRUE-1 site characterisation (before packer emplacement)			
Structural Investigations – tunnel mapping, geophysical surveys – borehole logging – core mapping	– fracture / rock classification – fracture statistics (orientation, frequency, width, trace lengths)	PNC/Golder	**++**
Geochemical Investigations – groundwater sampling – rock samples	– fracture / rock classification	–	**o**
Hydraulic Investigations – flow logging – single hole packer tests	– fracture transmissivity	CRIEPI, PNC/Golder, SKB/KTH-ChE, POSIVA/VTT, SKB/TRUE, Nirex/AEA	**++**
TRUE-1 site characterisation after packer emplacement			
Hydraulic Interference Tests	– transmissivity distribution and hydraulic connectivity (– hydraulic boundary conditions)	PNC/Golder, SKB/TRUE	**++**
Long-term Monitoring of Head	– hydraulic boundary conditions	PNC/Golder, SKB/TRUE, CRIEPI, POSIVA/VTT	**+**
Solute Tracer Tests (RC1)	– consistency check / system understanding	all groups	**+**

[1] Data improved the understanding of hydrogeological conditions at the site:
– data suitable for model discrimination / quantitative measures for model performance (++),
– data used to check the consistency of conceptual assumptions (+),
– complementary data with low impact on the conceptual model of groundwater flow (o).

Assessment of modelling tools (flow modelling) and convergence of approaches

Table 2-2 presents the spectrum of flow models applied by the modelling groups for Tasks 4A–D. Most of the groups used deterministic or stochastic continuum approaches, except PNC/Golder and SKB/KTH-ChE who applied a fracture network model and a channel network model, respectively. In all models, the flow equation was implemented in a Darcian formulation. A major limitation in most of the models was the 2D representation of the flow domain where Feature A was modelled as a homogeneous/heterogeneous 2D fracture. Exceptions are the models of BMWi/BGR (intersection of Features A and B implemented), PNC/Golder (3D fracture network) and SKB/KTH-ChE (3D channel network).

The modelling groups applied similar data sets for calibration/conditioning of their flow models. The database for calibration included:

- transmissivity values from single-hole packer tests,
- steady state / transient drawdowns during tracer tests,
- head values from long-term monitoring.

Hardly any of the groups (except SKB/KTH-TRUE) made explicit use of the interference test data. This fact may be explained by the limited resources of the modelling groups and by the focus on interpretation of the tracer test data (RC-1). On the other hand, there was an obvious lack of suitable tools for interpretation of interference tests. The diagnostic approaches described in ICR 96-04 / ICR 96-05 (normalised response time ratio, normalised drawdown ratio, reciprocity of test response) delivered a quite limited insight into the complex structure of the flow system. Furthermore, most of the modelling groups were restricted to 2D representation of the flow field at the site. Crosshole responses, however, showed clear responses across the features, indicating the need for a 3D structural descriptive model.

Various tools were used for calibration/conditioning of the models. CRIEPI estimated spatial distribution of transmissivity in Feature A by kriging from drawdowns observed in previously performed tracer tests (cf Figure 3-3a). Measured hydraulic heads before the tracer test were used to determine hydraulic boundary conditions. BMWi/BGR assumed a deterministic transmissivity distribution, homogeneous for Task 4C and for the later task a heterogeneous distribution fitted manually to the drawdowns observed in RC-1 (Figure 3-3b). SKB/KTH-TRUE conditioned their flow models with transmissivity and head values (undisturbed heads from long-term monitoring, drawdowns during RC-1, drawdowns during interference test 6). In addition, sensitivity analyses were carried out by varying correlation length of the T-distribution and by changing hydraulic boundary conditions. Figures 3-3c and 3-3d show two realisations.

Some of the modelling groups adopted the boundary conditions as they had been given in the descriptive conceptual model. The other teams calibrated/conditioned the boundary conditions with head values from long-term monitoring (e.g. PNC/Golder). In most cases, the process of model calibration was driven by resources and by the availability of geostatistical tool boxes rather than by careful assessment of data sensitivity (e.g. sensitivity analyses, perturbation analyses).

An evaluation of predictive flow modelling as part of Tasks 4C and 4D (radially converging and dipole tracer tests with conservative tracers) was accomplished in TR-99-04. One of the key finding of the evaluation was that prediction of drawdowns during tracer tests RC-1, DP-2 and DP-3 exhibited unsatisfactory results. The stochastic models of Nirex/AEA, SKB/KTH TRUE (unconditioned model) and PNC/Golder performed slightly better than the other models, however uncertainty of the stochastic models was quite large. In DP-2 and DP-3 (pumping in KXTT1), most of the models considerably underestimated drawdowns in the observation wells.

In conclusion, assessment of modelling approaches can be summarised as follows:

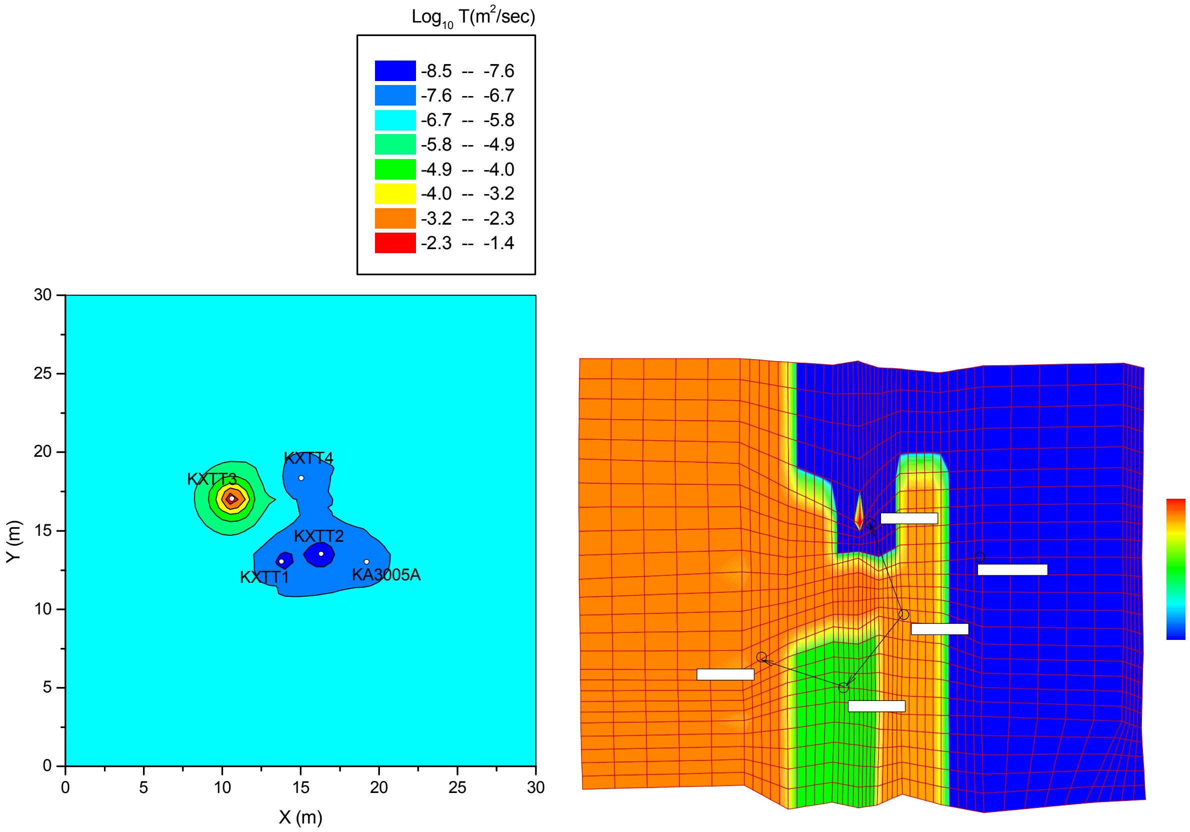
- A wide spectrum of model implementations was seen, ranging from homogeneous to heterogeneous transmissivity distributions and from simple to rather complex boundary conditions. This fact reflects the high degree of ambiguity associated with modelling of groundwater flow at the TRUE-1 site. In the course of the flow modelling tasks, convergence of the applied model concepts was hardly observed. It is concluded that groundwater flow at the TRUE-1 site is not understood well enough to perform predictive modelling for different boundary conditions.

- The stochastic models seemed to perform slightly better in predicting the drawdowns during tracer tests RC-1 and DP-1 to DP-3. Nevertheless, systematic misfits of drawdowns – especially in borehole KXTT2 – were seen in all modelling approaches, suggesting an incomplete understanding of the structures and hydraulic conditions at the TRUE-1 site. It is believed that the assumption of planar Feature A as a largely isolated planar element represents an oversimplification of the actual in-situ conditions.

- The fracture network model (PNC/Golder) proved to be an excellent tool for improving the conceptual understanding of groundwater flow at the site (cf Chapter 3.2.4). The tool is characterised by its great flexibility in handling a broad spectrum of geological and hydrogeological data (fracture statistics, flow logging, hydraulic interference testing, etc).

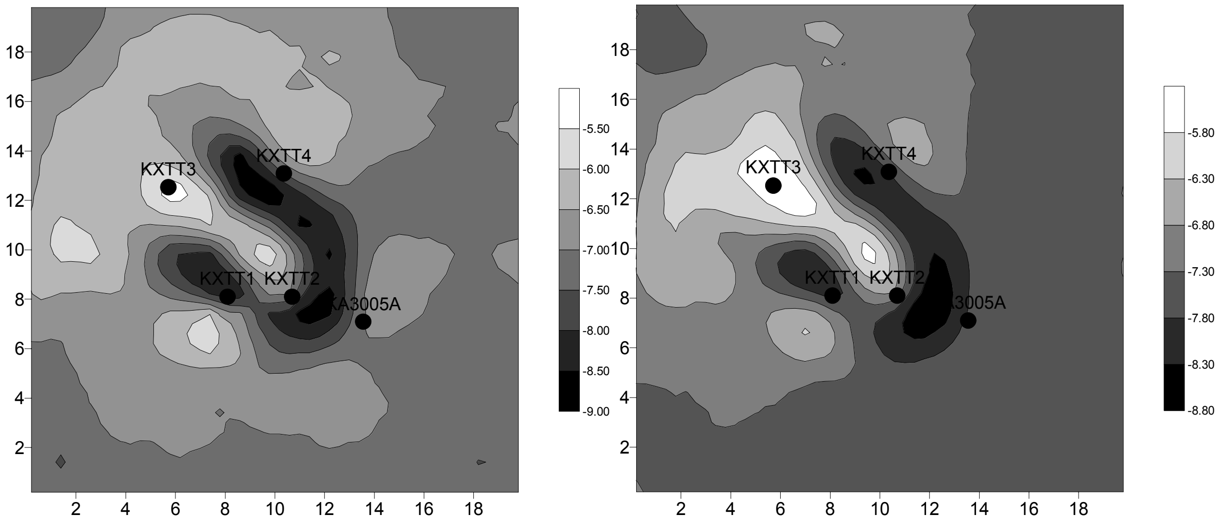
- Some of the transmissivity distributions are difficult to explain in a geological/hydrogeological framework. Thus, the rectangular shape of the heterogeneity in BMWi/BGR's model shows too strong an abstraction of reality. In CRIEPI's model heterogeneities in transmissivity are located concentrically around the monitoring boreholes, suggesting an artefact introduced by the calibration procedure. From a hydrogeological viewpoint, the stochastic SKB/KTH TRUE model represents a plausible transmissivity distribution in Feature A.

- Given the increasing amount of hydraulic data in the course of the TRUE-1 experiment (drawdowns during the tracer tests, long-term monitoring of hydraulic heads, hydraulic interference tests), careful re-analysis of the database would be desirable. In the context of the late stages of Task 4 priorities were given to the area of transport modelling. It is believed that a further interpretation of the existing hydraulic database by the modelling teams would lead to improved hydrological models of the site, which better account for the interconnectedness of the key hydraulic features.



a) CRIEPI transmissivity distribution.

b) BMWi/BGR.



c) SKB/KTH-TRUE conditioned on RC-1 data.

d) SKB/KTH-TRUE conditioned on RC-1 data with free boundary.

Figure 3-3. *Transmissivity fields applied by different modelling groups: (a) CRIEPI – stochastic continuum, (b) BMWi/BGR – deterministic continuum, (c) SKB/KTH-TRUE – conditional simulation on RC-1 data, (d) SKB/KTH-TRUE – conditional simulation on RC-1 data with free boundary.*

3.2.3 Understanding of transport mechanisms

The work within Task 4 focused more on radionuclide transport in the later tasks, Tasks 4C and 4D looking at transport of non-sorbing tracers and Tasks 4E and 4F also including transport of sorbing tracers. The inclusion of sorbing tracers added considerably to the complexity of the problem, greatly increasing the number of processes that potentially could be of importance. This led to an initial divergence in the modelling strategy of the different teams. However, as Tasks 4E and 4F evolved, the modelling groups tended to reach a more common viewpoint on the most important processes, although there were still considerable differences in the modelling approach.

Assessment of site characterisation data

The sorbing tracer tests were preceded by tests using non-sorbing tracers. For each of the two flow paths, results from six tracer tests with non-sorbing tracers were provided to the modellers. Thus, a large amount of data on hydrology and non-sorbing tracer breakthrough was available. These data were primarily used to derive flow velocities and dispersion coefficients, but were also analysed to arrive at reasonable values for other parameters. However, no tracer test data were available for calibration of the sorbing tracers. In that sense, the predictions made of sorbing tracer breakthrough can be considered as "blind".

Matrix interaction parameters were, to a large extent, given or suggested to the modellers, e.g. the modelling input data set (MIDS). This contained sorption coefficients, pore matrix diffusivities, matrix porosity and density derived from laboratory experiments on different rock materials from the Äspö site, such as fresh granite and weakly altered materials. Matrix sorption coefficients were primarily determined from through-diffusion experiments and diffusion penetration studies. If these were not available, results based on batch sorption experiments were given in the MIDS. The use of the MIDS data set and its application in the models was analysed only to a limited extent by the modelling groups.

However, several of the modelling teams established that altered material near the fracture surface or fault gouge material played an important role in the tracer retention. The lack of measurements on these materials restricted the possibilities of evaluation of the tracer experiments. Several of the modelling groups modified the given data in order to improve their predictions.

The site characterisation data did not contain any direct information on the relationship between the fracture surface area available for surface sorption and matrix diffusion (flow wetted surface) and the water flow rate. This ratio is of importance for the extent of interaction that will occur, but there are no established methods for measuring it in-situ. Thus, many of the modelling groups derived the value from the assigned geometric dimensions of the flow path (assumed width and aperture), which led to considerable variability between the groups.

In the analysis of the STT-1 and STT-2 pathway, it became apparent that breakthrough occurred along two distinct pathways with different transport properties. With the low pumping rate used in the STT-2 experiments this could be seen as a double peak. The existence of the double peak was revealed to the modellers after the submission of their predictions of Task 4F at the 12th Task Force meeting and was therefore only included in the final evaluation. Further evidence of dual pathways was found in the complementary experiments performed at the TRUE-1 site, see Chapter 2.1.5. The existence of the two distinct pathways complicated the modelling work for many of the groups, because of the increased number of parameters that needed to be assessed or because of difficulties in including multiple pathways in some of the models.

Assessment of modelling tools (transport modelling) and convergence of approaches

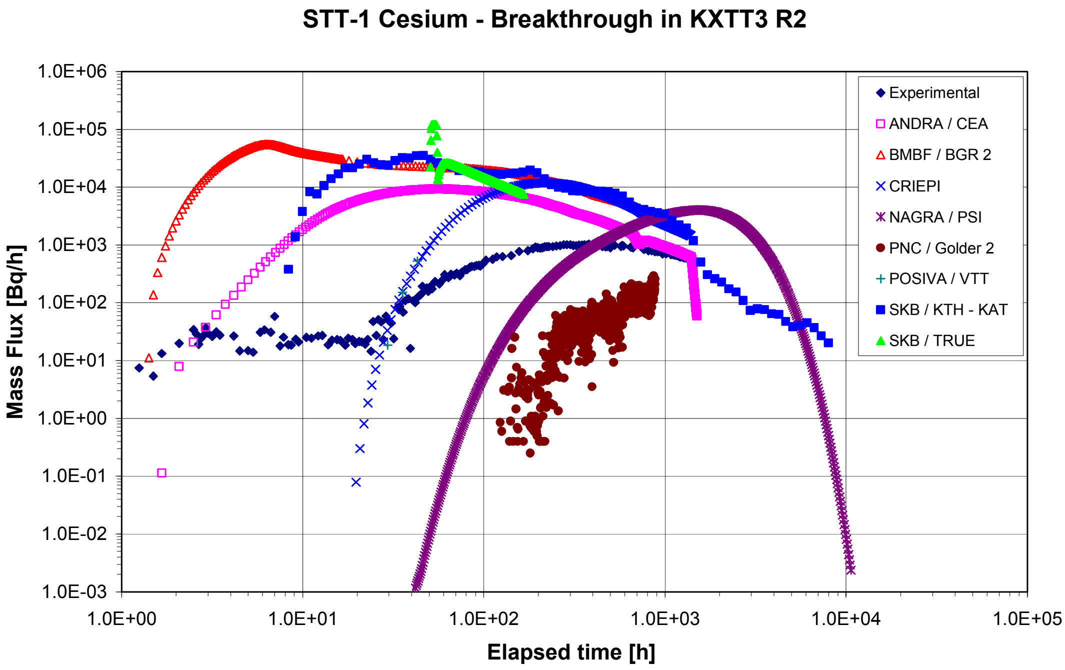
Tasks 4C and 4D focused on the advective and dispersive transport of non-sorbing tracers between boreholes intersecting Feature A. All modelling groups considered advection as the main process, with dispersion as a secondary process. Matrix diffusion was of very limited importance with the short travel times of the tracer experiments modelled within Tasks 4C and 4D.

The modelling groups were provided with very limited data on fracture aperture; instead apertures were derived from previously performed tracer tests. In order to satisfactorily simulate both the hydrology (drawdown) and transport (mean tracer breakthrough time) the relationship between hydraulic aperture and transport aperture of the feature needed adjustment. This was done either by independent calibration of transport aperture or by introducing scaling relationships between transmissivity and transport aperture. It was generally found that these relationships did not follow the cubic law.

There were considerable differences between the modelling groups in the way dispersion was implemented. A number of groups put the emphasis on effects of spatial heterogeneity and the presence of multiple flow paths, while other groups included dispersion as a Fickian-type of diffusion coefficient. However, the experimental scale and the injection source term used in the experiments modelled within Tasks 4C and 4D did not allow any discrimination between the results obtained with the two methods.

In Tasks 4E and 4F, the focus was on processes of importance for sorption, considerable development was made to take into account the effects of matrix diffusion and sorption, where both model parameters and model concepts were modified. For the initial simulations of STT-1 in Task 4E, the modelling groups based their models on results of preliminary design tests with non-sorbing tracers and the MIDS data set. When compared with the experimental results, it was found that the predictions of the sorbing tracer breakthrough in STT-1 were unsatisfactory. It was apparent that the involved processes were more complex than initially anticipated and that the application of laboratory data was not straightforward. As a result of model calibration and modification, the predictions were considerably improved for the later tracer tests (STT-1b and STT-2), compare Figure 3-4.

During the course of the exercise the models also became more similar in terms of what processes were considered, see Table 3-3. For the predictions of STT-2, matrix sorption and diffusion was included in all the models, whereas only half of the modelling groups used matrix diffusion and sorption in their predictions for STT-1. However, there were still substantial differences between how the processes were described in the different models used for the prediction of STT-2.



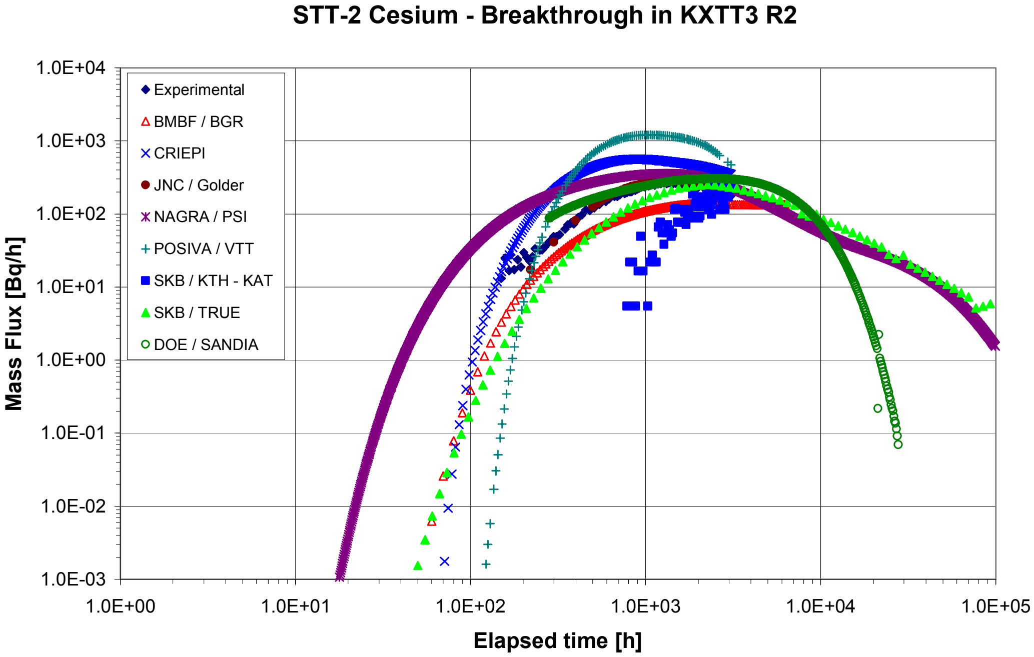


Figure 3-4. *Experimental results and model predictions of cesium breakthrough in Task 4E: STT-1 (upper) and Task 4F: STT-2 (bottom).*

Table 3-3. Summary of modifications made to take into account sorbing tracers.

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

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

To conclude, the assessment of modelling approaches can be summarised as follows:

- A wide range of modelling approaches has been applied for the transport modelling. Inclusion of relatively complex transport processes for the modelling of sorbing tracers has, in many cases, led to a need to simplify the geometric description of Feature A. Although the initial approach was very different, a general consensus on the processes to be included was reached for the predictions of STT-2, where all modelling groups included matrix diffusion and sorption. However, the description of the processes and their relative importance varied between the modelling groups.

- Most modelling groups found that sorbing tracer retention was underpredicted by a factor of 30–50 when directly applying the laboratory diffusion and sorption data. Several alternative explanations were given for this, see Chapter 3.3. However, with the present knowledge of the site it is not possible to determine the most plausible of these explanations.

- There are still a number of unresolved questions related to the application of data from laboratory studies and other sources in the modelling of tracer transport. This has a great influence on the predictive potential of the models. It is therefore not possible to draw clear conclusions on the predictive capabilities of the different mathematical models used within Task 4.

3.3 Interpretation methodologies

Introduction

It was a primary objective of this overall evaluation to highlight innovative and successful modelling approaches, developed in the course of Task 4 (cf Chapter 1.2). Recalling the fact that a total of 11 highly motivated modelling groups were involved for a time period of more than five years in the planning stages of the TRUE-1 experiment and in the interpretation of the test data, it is evident that a well balanced recognition of all methodological achievements and developments is beyond the scope of this evaluation. Therefore, the TRUE-1 overall evaluation team decided to select a few illustrative examples presented during previous Task Force meetings. The selection reflects a snapshot of the key interests of the Task Force team at various stages of Task 4. The following examples will be discussed in greater detail:

- The transport modelling approaches by SKB/KTH-TRUE, Nagra/PSI and SKB/KTH-ChE as part of Tasks 4E and 4F.

- The deconvolution approach presented by M. Elert during the 14th Task Force Meeting at Säröhus (IPR 01-30).

Further innovative studies will be brought to the reader's attention, even though they cannot be presented extensively in this report. Thus BMWi (ICR 98-02) and DOE/Sandia (ICR 99-02) adopted modelling approaches which had been developed and successfully applied in other investigation programmes (Grimsel, WIPP site). The application of these approaches (e.g. multirate diffusion, simplified dual-porosity concept) to the environment of the TRUE-1 site inspired the members of the other modelling teams and illustrated the spectrum of alternative conceptualisations of transport processes in fractured rock. CRIEPI (ICR 97-07) and the SKB/TRUE team (ICR 00-01) investigated innovative techniques for the calibration of flow and transport models. The modelling activities by Posiva (ICR 01-01), Andra and SKB/KTH-ChE (ICR 98-01) were primarily related to the needs of performance assessment. Various transport processes and upscaling mechanisms were implemented in simplified transport models (streamtubes, channel networks) and the performance of these code extensions was assessed in the context of the Task 4 predictive modelling exercises.

Approaches for evaluation of transport modelling

An important part of the Task 4E and 4F work was the evaluation done after the results of the experiment were revealed. The modelling groups put a lot of effort into the evaluation, calibrating model parameters, modifying and adapting models and testing alternative approaches. This has proved to be a successful strategy for evaluating the importance of different transport and retardation processes. The evaluation was to a large extent based on experience from related studies providing additional data that could be used to derive plausible explanations for the observations made in the TRUE-1 tests. A successful approach seems to have been to focus on critical issues and use simpler methods to evaluate the possible importance of various processes.

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

The Nagra/PSI team provides a good example of how geological information was used in the modelling evaluation. When setting up the model for prediction of the STT-1, the team found that the large amount of tailing observed in preliminary design test PDT-3 could not be explained by the low values of matrix diffusivity and porosity obtained from the laboratory measurements on Äspö diorite. A matrix form with considerably higher diffusivity and porosity must be present. Based on experience from the Grimsel site in Switzerland and structural geological investigations performed at Äspö, they concluded that presence of fault gouge could explain the breakthrough seen in the tracer tests, i.e. crushed and ground-up rock produced by friction between the two sides of a fault. However, no data were available for sorption and diffusion in the gouge material, and sorption was thus extrapolated from the measurements on Äspö diorite and the diffusivity evaluated from the breakthrough of non-sorbing tracers in previous tests. The initial predictions were good for non-sorbing and weakly sorbing tracers, but tended to overestimate the breakthrough time for the more sorbing tracers such as Rb and Cs. As a consequence of this, the interpretation of the geological model was revised and **flow-paths** also interfacing cataclasite were included for the predictions of STT-1b and STT-2. The approach used by Nagra/PSI was also adopted to some extent by other modelling teams, e.g. the SKB/KTH-TRUE and the Andra/CEA teams.

The SKB/KTH-ChE team found in their evaluation of the Task 4E and 4F experiments that the retardation caused by diffusion into the rock matrix and sorption within the matrix needed to be about 30 times larger then was obtained in the predictions based on the laboratory data. Several possible explanations for this were investigated. With the relationship used to model the matrix retardation effect, this implies that the product of the matrix sorption coefficient and the matrix diffusivity needs to be 900 times larger, or that the interaction area between the matrix and the flowing water needs to be 30 times larger. An evaluation of the sorption experiments was made considering also new data available on sorption on mylonite, altered Äspö diorite and altered fine grained granite.

The equilibrium sorption coefficients were estimated based on the fraction sorbed and the contact time of the batch sorption experiment. This resulted in matrix sorption coefficients that were 10–25 times higher for most tracers and 500 times higher for Cs. However, this increase was not sufficient to explain the difference between predictions and observations. It was further noted that the altered rim zone of the fractures was found to have an increased porosity. Values between 2–3% were estimated for the part of the zone accessible to the tracers during the tests. This would imply a matrix diffusivity 10–20 times larger than measured in the rock mass. An alternative explanation would be if the flow rate in the transport path was less than predicted or if the ratio flow-wetted surface to water flow rate was considerably larger. This could be the case if there is an uneven flow distribution around the extraction section, with a high transmissivity zone conducting most of the water pumped in the extraction section. There are indications of a highly conductive zone between KXTT2 and KXTT3. Water from the injection sections may thus travel long distances in Feature A in low flow rate paths before entering the extraction hole or the highly conductive zone. Simulations carried out in two-dimensional fractures indicate that a flow rate a factor 5–10 lower is possible.

Deconvolution approach

It was recognised early during the work in Task 4 that the shape of the tracer injection curve interfered with the interpretation of the breakthrough curve. Although the injection methodology was improved during the course of the TRUE experiments, the “hump” appearing after the second flushing of the injection section was large enough to influence the breakthrough at late times. A way to circumvent this problem is to use deconvolution techniques. Such mathematical techniques can be used to analyse linear systems where the output function is given by an input function and a unit response function. For a tracer test, the unit response function describes how the breakthrough curve would look like if the injection curve was a Dirac delta function, i.e. a pulse with unit mass and zero duration. Thus, the unit response function describes the characteristic features of the particular flow and transport problem, removing the effects caused by the injection curve. The unit response function can then be used to evaluate and characterise the transport mechanisms along the flow path.

Deconvolution was performed of the experimental results of the tracer tests STT-1 and STT-1b (IPR 99-35) and STT-2 (IPR 00-22). Unit response functions were derived from the experimental injection and breakthrough curves using the Toeplitz method. Since deconvolution is an ill-conditioned problem, where small experimental errors give rise to oscillations, various types of filtering were necessary. However, oscillations in the tails of the breakthrough curves were still apparent in many cases. In general, the tail of the unit response function could be traced 2 to 2 1/2 orders of magnitude below the peak value. In order to have a good resolution of the initial breakthrough for the non-sorbing tracers, a smaller time step was needed than was found to be numerically stable with the applied deconvolution method.

Deconvolution was used only to a limited extent in the evaluation of Tasks 4E and 4F. The double peak found in the breakthrough curve of the STT-2 experiment remained in the unit response curve obtained from the deconvolution. This was taken as an indication that the double peak is not an artefact of the injection procedure, but is due to the presence of multiple pathways in the tracer test. The analysis made of the late time behaviour of the unit response curve from the STT-2 experiment indicates a slope of the tail of roughly –3/2 in a log-log scale, which would be characteristic of the matrix diffusion and sorption processes. No saturation of the matrix was indicated for the time period covered by the unit response curve (~1000 hours).

Deconvolution techniques have a potential for obtaining unit response curves that can be used for evaluating tracer tests with injection curves that are non-ideal from a modelling point of view. Many of the mathematical models used within Task 4 derived unit response functions as a part of the transport calculations. A comparison between unit response functions predicted by models and those derived from the experimental data gives information on how well the models describe the actual transport processes. Increased use of unit response curves derived from the experiments should be considered for the evaluation of modelling future tracer experiments. However, further development of the present method is needed in order to obtain a better resolution of non-sorbing tracer breakthrough and to handle curves with large experimental errors.

3.4 Steering aspects

3.4.1 Overview

The Task Force Charter (revised version, presented at the 6th TF Meeting in Västervik 1995) represents the overall framework for managing the Task Force. The Charter defines in a general way the purpose of the Task Force forum, the role of the team members and their responsibilities and, finally, the scope of the Task Force as part of the Äspö Project.

Beyond the general rules set out in the Charter, a set of purpose-oriented steering tools was adopted by the TF Chairman to run the different tasks. In the framework of the Task Force meetings, the appropriateness and success of the applied steering tools was jointly evaluated by the TF Chairman and the TF Delegates. Task steering had to deal with the following aspects:

- to motivate the modelling groups and assist them in executing their tasks,
- to assess the technical output of the modelling teams in a structured and traceable way,
- to address the administrative requests by SKB and by the other participating organisations.

The key steering elements employed in the course of Task 4 include the periodic Task Force meetings, a formalised procedure for task definition and, finally, a rigorous documentation of achievements with well established levels of reporting (Table 3-5). It is the aim of this overall evaluation of Task 4 to highlight these steering tools and to assess their success from the viewpoint of the experiment delegates. Evaluation is focused on the following criteria:

- contribution to the overall aims of Task 4 as defined in Chapter 2.3,
- motivation/challenging of the modellers.

Table 3-5. Key steering elements employed in the course of Task 4.

Steering Elements	Features
Periodic TF Meetings	– Progress and Task Evaluation Sessions – Modeller's Sessions / Executive sessions – Wrap-Up sessions
Task definition and task management	– Agreed TF Charter – Formalised Task definition – Definition of expected deliverables – Formalised distribution of data base – Action lists – Performance measures (Prediction / Evaluation tasks) – Questionnaires – Summary tables of modelling approaches – Task evaluation reports
Reporting	– Handouts / Proceedings of the TF-Meetings – ICR and SKB Technical Reports – Papers in scientific journals

3.4.2 Periodic Task Force meetings

General aspects

Task Force meetings were held every 6 to 9 months. The meetings were hosted alternately by SKB and one of the other participating organisations – a feature which was appreciated by the TF members as an opportunity to learn more about the radwaste programmes of the different organisations. According to the scope of the prevailing subtasks, the meeting dates were fixed to be flexible enough to account for both the requirements of the Äspö Project (input for TRUE-1 project team) and the resources of the modellers.

Only in the early stages of Task 4 (7th and 8th TF meeting in Hergiswil and Hultsfred) did the modelling teams seem overstretched by the extent of the Task 4B and 4C work programme – the tight task schedule was strongly driven by the wish of the Task Force team to provide input to the TRUE-1 field programme. Due to the enormous progress of the TRUE-1 project team, however, the Task Force had to accept that it was impossible to keep pace with the in-situ experiment. As a consequence, the modellers' input to the experimental design (Task 4B) was delivered too late to feed into the TRUE-1 test plan. In later stages of the Task 4 programme, subtask definitions and allocated timeframes were generally well balanced.

Organisation

The main purpose of the Task Force meetings was to evaluate the accomplishments of the modelling groups. A standardised task evaluation procedure was implemented, consisting of:

- progress and evaluation sessions,
- simultaneous executive sessions and modellers sessions,
- task wrap-up sessions.

The *task progress and evaluation sessions* were aimed at reviewing the progress of the modelling teams. Each modelling group presented the accomplishments of the previous modelling period and highlighted their key findings. A strict order of presentation was not requested, except for the predictive modelling exercises: in the context of predictive modelling, a predefined format of the expected modelling output was requested to ensure the comparison of the modelling results with the field data. Subsequent to the presentations, a brief evaluation of the modelling results was initiated by the TF chairman. Both modelling groups and Task Force members contributed to the discussions.

The progress and evaluation sessions formed the platform for the modellers and for the TRUE-1 project team to interact with each other. Modellers were able to compare modelling approaches and to learn about implementation of the approaches in their colleagues' codes. Little emphasis, however, was given to the technical review of the contributions – sometimes the modelling groups may have missed technical feedback and scientific guidance by the TF delegates.

Modellers' sessions and *executive sessions* were held simultaneously. A session chairman was appointed for the modellers' sessions. His task was to work jointly with the modellers on a specific topic (e.g. elaboration of questionnaires, proposal for future tracer tests, definition of data requests) and, finally, to report the accomplishments of the team to the TF delegates. The executive sessions, consisting of the TF chairman and the TF delegates, formed the actual steering board. The TF delegates discussed openly their opinion about the current status of the task and expressed the wishes of the participating organisations for future tasks. Within the executive sessions, the task definitions, task procedures and expected deliverables of the modelling groups were approved. Finally, the decisions were communicated to the members of the modelling groups and the TRUE-1 team, respectively.

Modellers' sessions and executive sessions turned out to be a successful means for stimulating the TF members to active participation. Due to the informal character of the sessions, both modelling team members and TF delegates felt encouraged to discuss scientific and administrative issues beyond the actual task scope. In this context, the role of the session chairmen is to be emphasised. The success of the modellers' sessions and executive sessions was ensured by well prepared chairmen, who were able to summarise concisely the main output of the meetings and to communicate the achievements at the subsequent plenary sessions.

Wrap-up sessions were aimed at summarising the actual task status, to defining new subtasks and approving the requested deliverables towards the next TF meeting. At the end of a wrap-up session an action list was generated, specifying the expected deliverables, responsibility and the deadlines.

3.4.3 Task management

Since the early stages of the Task Force, a traceable procedure has been developed to define, implement and operate new tasks – and finally, to evaluate the accomplishments. Task 4 has been one of the most complex tasks so far and is representative of the iterative refinement of task management in the course of the Task Force. A whole series of typical steering elements is listed in Table 3-5. Subsequently the task management procedures are discussed according to the different (sub)task stages:

- formalised (sub)task definition,
- standardised task procedure,
- task evaluation procedure,
- reporting (cf Chapter 3.4.4).

Task definition

New tasks and subtasks were initiated in a formalised way through a *written task proposal*, which consisted of a short scope, *definition of objectives*, description of the data base, tentative schedule and a definition of the expected output. Generally, (sub-)task proposals were launched by the TRUE-1 project manager (A Winberg) – the proposals were presented and discussed in TF plenary sessions and approved by the TF delegates (executive sessions). In the executive sessions, the TF delegates confirmed participation of their organisations and *nominated their modeller groups*.

Excellent task definitions by the TRUE-1 project team provided a reliable basis for the modelling teams to estimate the required resources. For the TF delegates, the task proposals formed the key document to justify to their organisations the participation of their modelling groups in a subtask. Last but not least, as part of the task evaluation process the detailed specification of objectives and expected deliverables facilitated a traceable back-analysis of achievements. Therefore, the structured procedure of setting up the new (sub-)tasks was appreciated by both modellers and TF delegates.

Task procedure

Obviously, the evolution of Task 4 was largely driven by the progress of the TRUE-1 experiment. The TF meetings were scheduled in close coordination with the experimental milestones. As part of each TF meeting, an updated task schedule was elaborated and documented during the wrap-up sessions (*action list*). The requested deliverables and the deadlines were discussed and jointly agreed by all TF members – hence, the committed action list represented a simple, but nevertheless effective management tool for the TF chairman to survey the progress of the prevailing task.

Elaboration and distribution of *data packages* by the TRUE-1 project team had a great impact on the progress of the modelling work. In particular for the predictive modelling exercises (Tasks 4C–F), the data packages represented the key input for building the numerical models, for defining the modelling strategy and for the subsequent model predictions and model analyses. Various types of data were distributed (e.g. descriptive conceptual models, interpreted test data, pressure / flow transients, breakthrough curves). In the early stages of Task 4, distribution was carried out by mail or email, more recently download areas were established on SKB’s website, allowing for convenient and quick access to the latest data deliveries.

Generally, the data distribution was organised very well and did not give rise to any notable criticism by the modellers. The structure of the data deliveries was clearly arranged and the deadlines for data distributions were met.

Several data packages contained contributions to the descriptive conceptual model of the TRUE-1 site. These contributions reflected the prevailing conceptual site model as elaborated by TRUE-1 project team. It is worth mentioning that many of the modelling groups used these data as “hard” facts without assessing the inherent uncertainty of the basic conceptual assumptions. Similarly, most of the modellers made use of interpreted field test results (e.g. transmissivity values from packer tests) rather than analysing the raw data with their own models. As a consequence, in some subtasks the model predictions of the different modelling groups showed a degree of consistency which did not reflect the real uncertainty of the problem under investigation (e.g. general overprediction of drawdown during RC-1 / cf TR-99-04).

Task evaluation

Achievements of the subtasks were assessed during the progress and task evaluation sessions (cf Chapter 3.4.2) and documented in so-called task evaluation reports (TR-99-04, TR-01-12).

Summary tables of the adopted modelling approaches were elaborated as part of the modellers’ sessions. For the TF delegates these tables turned out to be a valuable means for comparison of codes and modelling strategies. Worth mentioning is a comprehensive overview of flow and transport modelling approaches, elaborated as part of the Task 4C and 4D evaluation report (TR-99-04). In the present report, those descriptions are given in Tables 2-2 and 2-3 in a more condensed form, addressing the type of model used, description of the modelled processes and a brief characterisation of model geometry and model parameters, respectively.

Questionnaires were used to establish the modellers’ view of the task definitions. The questionnaires scrutinised the scope and issues of participation of the modelling teams. Technical problems were highlighted (conceptual model, data base, boundary conditions, calibration and conditioning, sensitivity analysis). Interpretation of the modelling results, assessment of process understanding, lessons learned, open issues and recommendations were further aspects of interest.

The modellers’ answers to the questionnaires may be seen as snapshots, indicating the level of maturity in process understanding at different stages of Task 4. A good example is the questionnaire concerning Tasks 4C and 4D (TR-99-04) – it reflects the high degree of conceptual uncertainty the modellers faced in the early process of model implementation. At this stage, the modellers preferences for certain types of data are still driven by the capabilities of their modelling tools and a wide spectrum of different approaches is used to implement the descriptive conceptual model. For the modelling teams, the questionnaires may have served as an opportunity to perceive the common ground of the different conceptual approaches and, hence, to improve the internal consistency between the approaches.

For each of the prediction/evaluation tasks (Tasks 4C–F) a set of *performance measures* was defined to evaluate the accuracy of model predictions and to compare the results of the different modelling approaches. Definition of suitable performance measures was a joint action of the modellers and the TRUE-1 project team (modellers' sessions). Drawdowns in monitoring boreholes, median tracer breakthrough times or total mass recovery during tracer testing are typical examples for performance measures. The modelling teams had to provide their modelling results in a predefined data format, such that the performance measures could be easily compiled and compared. Within the framework of special progress and evaluation sessions the TRUE-1 project team reported their experimental results and compared them with the predictions of the modellers.

The prediction/evaluation exercises created great excitement and – in a positive sense – an atmosphere of competition among the modellers. The quality of the different model predictions was intensively discussed – the performance measures served as the key criteria for assessment of the model predictions. Apart from the quantitative performance measures, simple diagnostic analyses proved to be another valuable means for qualitative evaluation of the model predictions. For example, tracer breakthrough curves were plotted not only in cartesian coordinates but also in semi-log and log-log representations, which allowed a better decomposition of the predicted early time and late time behaviour (advective and diffusive transport processes).

Task evaluation reports are the final step in the evaluation process. In the course of Task 4, two subtask evaluations were written (TR-99-04: Evaluation of Tasks 4C and 4D; TR-01-12: Evaluation of Tasks 4E and 4F), completed by the present Task 4 Overall Evaluation Report. The reports were produced by external reviewers and/or by TF delegates, summarising in a concise way the modelling results and the task evaluation process (adopted modelling approaches, questionnaires, performance measures).

3.4.4 Reporting

Reporting was an issue of vital importance for SKB, but also for the other participating organisations – mainly driven by the need to demonstrate the progress of the Task Force's mission. Different types of documents were requested by the TF secretariat:

- Handouts of the modellers' presentations (distributed during the TF meetings).
- Minutes of the TF meetings (International Progress Reports).
- Task reports of the modelling teams and the TRUE project team, respectively (International Cooperation Reports).
- Task evaluation reports (SKB Technical Reports).

In addition, all modelling groups were encouraged to submit manuscripts of their modelling activities to scientific journals for publication.

In the course of Task 4, more than 15 task reports were written by the modelling teams. Since the 6th TF Meeting in Västervik (June 1995), a vast amount of supplementary technical information has been compiled in the minutes of the TF meetings, including the various subtask definitions, handouts of the modellers' presentations and summaries of the evaluation sessions. On the other hand, the number of scientific papers produced in the framework of Task 4 was rather low.

The fact is that reporting was not the favourite activity of the modelling teams – in particular the ICR reports turned out to be demanding job. In the early stages of Task 4, the deadlines defined during the wrap-up sessions seemed to be too tight for some of the modelling groups, overstretching their resources and eventually leading to major delays in the date of report delivery. Towards the later stages (Tasks 4D–F) a clear improvement was seen in the delivery time, but also in the structure of the reports. This includes detailed descriptions of the test site and the field experiments, a traceable summary of the applied modelling tools and, in particular, a standardised presentation of the modelling results. Those who were involved in the task evaluation process appreciated the increasing quality of the task reports.

Even in the later stages of Task 4 it was felt that reporting largely absorbed the modellers' resources – maybe this is the reason why the number of publications was so low.

4 Conclusions and outlook

4.1 Conclusions

4.1.1 Lessons learned

Modelling of groundwater flow

Modelling of groundwater flow was a focal point in the early stage of Task 4 (Tasks 4A–D), a period which was characterised by many conceptual and technical uncertainties: the structural descriptive model of the TRUE-1 site was still under development, the modellers were confronted with a vast amount of site characterisation data and the layout of the site instrumentation was still in a process of iterative refinement (e.g. packer locations, tracer injection systems). In that stage of incomplete understanding of groundwater flow conditions at the site, the modelling teams had to choose the appropriate modelling tools and to define the outline of the modelling strategy.

Five of eight modelling teams used a 2D model geometry to work on Tasks 4C and 4D (cf Table 2-2). This choice turned out to be a major restriction in the process of data analysis and model calibration, which was particularly seen in the interpretation of the hydraulic interference tests – the complex crosshole responses clearly indicated the need for a 3D structural descriptive model. At the end of Task 4D, when an extensive site characterisation data base was available and the instrumentation of the TRUE-1 boreholes had been completed, increasing priority was assigned to transport modelling. For this reason, the modelling teams did not have the time to reconsider their tools for flow modelling and to revise the modelling approaches. As a consequence, the understanding of groundwater flow conditions at the site remained incomplete, despite the excellent site characterisation data available. With a view to future prediction/evaluation tasks, the allocation of time for comprehensive model revision may be desirable as the final step in the task procedure.

The structural investigations provided the basic site characterisation data needed to establish the structural descriptive model. Pressure monitoring during drilling and flow logging in the newly drilled TRUE-1 boreholes was of great value for the determination of the hydraulic connectivity of the fracture systems at the site and for the choice of packer locations. Among the wide spectrum of site characterisation data provided by the TRUE-1 project team (cf Chapter 3.2.2), packer testing, long-term monitoring of hydraulic head and solute tracer tests represented the most attractive information for the modelling teams. Geochemical investigations for fracture classification provided complementary information for model refinement.

Golder's Fracman/MAFIC turned out to be an excellent tool in the process of establishing the structural descriptive site model. The inherent flexibility of the stochastic fracture network approach, but also the fracture network visualisation capabilities and the wide spectrum of data analysis modules (e.g. fracture statistics, hydrotest analysis, flow logging), allowed for a balanced integration of the different types of site characterisation data.

A wide spectrum of flow modelling approaches was seen in Task 4, including 2D and 3D representations of the site, stochastic and deterministic approaches and homogeneous and heterogeneous distributions of hydraulic properties. At the end of the flow modelling exercise, a consistent picture of the hydraulic conditions at the site was not achieved. Some of the modelling groups explained the flow field by introducing complex boundary conditions, other groups focused on heterogeneous distributions of hydraulic properties at the site. Systematic misfits of drawdowns were seen in the Task 4C and 4D drawdown predictions of all modelling groups – it is concluded that the understanding of groundwater flow at the TRUE-1 site is still incomplete.

Modelling of radionuclide transport

A general consensus as to the most important transport processes developed between the modelling groups during the work within Task 4. Although the same general processes are included in all the models, there are considerable differences in how they are modelled and the emphasis put on individual processes.

Very different approaches can, to a reasonable degree simulate the breakthrough curves obtained from the TRUE-1 tracer tests and also with the available information make reasonable predictions. However, these predictions have not been entirely “blind” as results from previously performed tests have been used to calibrate the models.

Transport of radionuclides in fissured rock is governed by a number of processes that to a great extent interact with each other. Many of the processes (matrix diffusion and sorption, diffusion into stagnant zones, hydrodynamic dispersion, sorption kinetics) have very similar effects on the breakthrough curves obtained from tracer experiments and cannot be discriminated in a single breakthrough curve. Experiments involving several tracers with different sorption properties can to some degree be used to distinguish between some of the processes, but due to experimental uncertainty, limited resolution in the tail end of the breakthrough curve, etc, a definite distinction between processes cannot be made. Therefore, the understanding of radionuclide transport in a fissure has to rely on a combination of information from many types of sources, field observations, laboratory experiments, theoretical studies, etc. Modelling work is an important part of evaluation and integration of this information since it provides the possibility to test various phenomena and processes that may be of importance.

When setting up models for complex transport processes occurring in heterogeneous media, it is necessary sometimes to make simplifications. In general, transport models focus on transport processes and tend to use as simple a geometric description as possible, e.g. modelling, transport along a one-dimensional streamline. The results of the Task 4 modelling, indicate that this approach is sufficient for making reasonable simulations of radionuclide release. However, the results also show that there are still issues that need to be resolved before reasonably accurate “blind” predictions can be made and that questions still remain concerning the extrapolation of simulations to other spatial and temporal scales.

A modelling exercise such as the Äspö Task Force on Modelling of Groundwater and Transport of Solutes provides a unique forum for modellers with different background and experience to come together and focus on a common problem. For radionuclide transport modelling, this possibility of interaction is of great importance for increasing the understanding of relevant processes.

The modelling groups were provided with extensive background material covering geostructural models, hydraulic testing, preliminary tracer tests and laboratory measurements. It must further be acknowledged that the modellers had limited resources to perform the Task Force work, due to the work being done in parallel with research for national programs. Thus, this extensive background material has not always been analysed in full detail.

4.1.2 Unresolved issues

Modelling of groundwater flow

Among the modelling teams involved in Task 4, no real consensus was reached on the description of groundwater flow conditions at the TRUE-1 site, despite the great amount of available site characterisation data. The wide spectrum of applied modelling approaches reflects well the conceptual uncertainties the modellers had to deal with. Possible sources for those uncertainties are:

- The structural descriptive model, elaborated by the TRUE-1 team (cf Chapter 2). The structural model assumes that the TRUE-1 site is made up of a small number of more or less planar hydraulically relatively well isolated features. In the course of Task 4, refinements of the structural descriptive model were released. Alternative structural models, however, were not assessed.

- The instrumentation of the boreholes. If the packer locations are not appropriately selected, the borehole intervals may distort the groundwater flow system at the site by short-circuiting the different hydraulic features. In the course of Task 4, a rearrangement of the packer systems was made prior to the tracer test RC-1.

- Inappropriate modelling approaches (e.g. 2D representation of the site).

- The tight task schedule, which did not provide the time needed for comprehensive model revisions.

A consistent picture of the hydraulic property distribution at the site, and of the characterisation of the interconnectedness of the fracture systems, was not achieved. Similarly, the hydraulic boundary conditions remained uncertain.

Modelling of radionuclide transport

The work within Task 4 has highlighted several points that not are completely resolved concerning the understanding and modelling of radionuclide transport:

- Uncertainty arises from the inherent fact that the properties of the actual flow paths within the tested feature are to a large extent unknown. This concerns for example the number of independent flow paths, the width of the flow paths, the minerals on the fracture surfaces, the properties of the rim zone and the occurrence of fracture infilling. This affects important parameters such as the flow wetted surface, the possibility for diffusion into stagnant zones, the extent of matrix diffusion and sorption. It must be recognised that complete knowledge of flow paths in fractures cannot be obtained, but a greater understanding of their general properties is needed in order to make predictions of radionuclide transport.

- Many of the important transport and retardation parameters can only be measured in situ with great difficulty and cost. Therefore, measurements on samples in the laboratory are needed. The work within Task 4 has shown that the transfer of laboratory data on matrix diffusivity and sorption to models for field experiments is not completely straightforward. This is largely due to the heterogeneity in rock type along the flow path, but also due to heterogeneity within the rim zone of the fracture. These uncertainties have strong implications for the use of data in performance assessment modelling.

- The detailed characterisation of the site that is planned after the end of the test period, e.g. resin injection followed by excavation of the feature, can be expected to provide valuable information on the geological structure of Feature A and the flow paths used for the tracer experiments.

4.2 Outlook

After completion of Task 4, a number of unresolved issues has been identified concerning flow and transport processes at the TRUE-1 site. Furthermore, the Task Force members learned a lot about effective task management. At the end of this overall task evaluation process, it is the intention of the authors to direct the thinking of both the Task Force and of the TRUE-1 project team towards innovative suggestions in support of future field investigations and modelling tasks. Recommendations and suggestions emphasise the following issues:

- The structural descriptive model is a basis for understanding flow and transport. Geological and hydraulic data do not provide a unique conceptualisation of the site, particularly concerning the connectivity of the involved features. We therefore believe it is very fruitful for the Task Force to encourage the testing and elaboration of alternative hypotheses. In this context, it is worth mentioning that alternative conceptualisations and models were developed in conjunction with Task 4, especially concerning the tracer retention observed in sorbing tracer tests. These will be the subject of further investigations in the following Task 6.

- In the course of the TRUE-1 project, refinement of the instrumentation arrangement was made. The modification was based on the prevailing structural descriptive model. Given that alternative descriptive models will be assessed in future, a revision of the actual instrumentation arrangement may be required to address the characteristic features of the alternative models.

- The modelling teams have had access to a large amount of data concerning the TRUE-1 site. To some extent raw data has been provided, e.g. results of interference tests, but a large amount of data consisted of processed data, e.g. evaluated transmissivities and the MIDS data set for radionuclide diffusivities and sorption. Delivery of a structural descriptive model and of further processed data by the TRUE-1 project team has been necessary in order to achieve the amount of modelling performed within Task 4 with the limited resources available. However, the data processing is based on model concepts and assumptions and is therefore closely linked to the modelling process. It is therefore proposed that the Task Force encourage independent data processing by the modelling teams, e.g. by suggesting performance measures consisting of intermediate results.

- Interference tests are a particular source of hydrogeological information, that were not analysed in depth by the modelling teams. Seemingly, the main reason was the lack of appropriate (stochastic) 3D flow modelling tools needed to interpret the complex pressure responses. In addition, a comprehensive interpretation methodology was not available – with the exception of some diagnostic analyses presented by the TRUE-1 team. It is therefore recommended to establish a future modelling (sub-)task, which is aimed at developing strategies for interference test interpretation in fracture networks. The TRUE-1 structural descriptive model in combination with the vast amount of field data may provide an ideal data base to develop and test such a methodology.

- At the end of Task 4D, priorities were clearly set for transport modelling – hence, the modelling teams did not have enough time to revise their groundwater flow models. With a view to future modelling tasks, it is strongly recommended to allocate sufficient time for a comprehensive revision of the predictive models in the final stage of a prediction/evaluation task.

- The results of the Task Force work need to reach a wider audience than the readers of the Task Force reports. It is therefore important to encourage the modelling teams to write scientific papers. In order to achieve this it may be necessary to allocate resources for writing papers (e.g. reduce the workload for ICR / SKB TR reporting).

- Working group sessions turned out to be a very creative element in the course of the TF meetings. The modelling teams had a chance to interact with each other in an informal manner, talking about problems beyond the immediate focus of the actual modelling task. It is proposed to intensify the topical discussions on technical issues in the framework of working group sessions (e.g. comparison of discretisation problems in different numerical approaches).

- Sometimes, a lack of technical feedback to the modellers was seen during the evaluation sessions. Topical evaluation sessions with external reviewers are recommended to initiate more lively technical discussions. A clear definition of the evaluation issues and a careful selection of the external reviewers is a prerequisite for the success of such topical evaluation sessions.

- The executive sessions offered an opportunity for the TF delegates to pinpoint the specific interests of their organisations and to participate actively in the process of task definition. The informal sessions created team spirit and encouraged the members to feel responsible for the overall missions of the Task Force. It is recommended to revive the executive sessions as a valuable steering tool.

5 Overview of reports

This section lists the reports prepared within the Äspö Modelling Task Force for modelling Tasks 4. It also lists the relevant Äspö reports used as references in the Overall Evaluation.

Äspö International Cooperation Reports

ICR 96-04	First TRUE Stage – Tracer Retention Understanding Experiments. Descriptive structural-hydraulic models on block and detailed scales of the TRUE-1 site. SKB TRUE Project Team, PNC/Golder Team, USDOE/LBNL Team, A Winberg (editor), Conterra AB, May 1996.
ICR 96-05	Discrete fracture analysis in support of the Äspö Tracer Retention Understanding Experiment (TRUE-1). W Dershowitz, A Thomas. R Busse (Golder Associates, Inc), April 1996. Supported by PNC, Japan.
ICR 97-02	Tracer Retention Understanding Experiments (TRUE). Test plan for the TRUE Block Scale experiment. A Winberg (Conterra AB), November 1996.
ICR 97-07	Numerical analysis with FEGM/FERM for TRUE-1 non-sorbing tracer tests. Y Tanaka, T Hasegawa, M Kawanishi (CRIEPI), October 1997.
ICR 98-01	Modelling of the Tracer Retention Understanding Experiment Task 4C–D using the channel network model. B Gylling, B Khademi, L Moreno (KTH), January 1998.
ICR 98-02	Modelling of tracer experiments in Feature A at Äspö HRL. L Liedtke, H Shao, Federal Institute for Geosciences and Natural Resources (BGR), Hannover, Germany, Supported by BMBF, August 1997.
ICR 98-03	Modelling of the tracer tests in radially converging and dipole flow fields in the first phase of the TRUE project. Antti Poteri (VTT Energy), Aimo Hautojärvi (Posiva OY), Supported by Posiva OY, June 1998.
ICR 98-06	Modelling TRUE-1 (RC-1) tracer tests using a heterogeneous variable aperture approach. Äspö Task Force, Task 4C. W Worraker, D Holton and KA Cliffe (AEA Technology, Supported by UK Nirex), March 1998.
ICR 98-07	Prediction of the TRUE-1 radially converging and dipole tracer tests. Äspö Task Force, Tasks 4C and 4D. J-O Selroos, SKB, V Cvetkovic (KTH), August 1998.

ICR 99-02	Solute transport modelling of the Äspö STT1b tracer tests with multiple rates of mass transfer, Task 4E. S McKenna (Sandia National Laboratories, USA), February 1999.
ICR 99-03	Modelling the reactive-radioactive and sorbing tracer tests in fractured rock, Task 4E and 4F. H Shao and L Liedtke (BGR) October 1999.
ICR 00-01	First TRUE Stage evaluation of tracer retention understanding experiments (first stage) at Äspö. V Cvetkovic, H Cheng (KTH), J-O Selroos (SKB), August 1998.
ICR 01-01	Modelling of the TRUE-1 sorbing tracer tests. Äspö Task Force, Task 4E and 4F. A Poteri, VTT Energy, Supported by Posiva Oy, May 2000.
ICR 01-02	Tracer tests with sorbing tracers.Task 4E-I:SST-1 Blind prediction. Task 4E-II: Analysis of STT-1 blind prediction. Task 4E-III: Predictions for STT-1b. Task 4F: Prediction for SST-2. Äspö Task Force, Task 4E and 4F. W Dershowitz, T Cladouhos (Golder Associates Inc), M Uchida (JNC), January 2000.
ICR 01-03	Evaluation of sorbing tracer tests using the channel network model. Äspö Task Force, Task 4E and 4F. L Moreno (KTH), August 2000.
ICR-01-04	First TRUE Stage – Complementary investigation of diffusivity, porosity and sorptivity of Feature A-site specific geologic material. J Byegård, H Widestrand, M Skålberg (Chalmers University of Technology), E-L Tullborg (Terralogica AB), M Sittari-Kauppi (U of Helsinki), April 2001.
ICR 01-05	Simulation of the Äspö tracer retention understanding (TRUE-1) experiment, Radially converging and dipole tracer experiments. Äspö Task Force, Task 4C and 4D. W Dershowitz, T Eiben, R Busse, I Kluckow, P Wallman (Golder Associates Inc), January 2000.

Other Äspö reports

HRL 96-24	TRUE 1st stage tracer test programme. Experimental data and preliminary evaluation of the TRUE-1 radially converging tracer test (RC-1). Anderson P (Geosigma), Äspö Hard Rock Laboratory Progress Report.
IPR 99-35	Deconvolution of breakthrough curves from TRUE-1 tracer tests (STT-1 and STT-1b) with sorbing tracers. Äspö Task Force, Task 4E. M Elert, H Svensson (Kemakta Konsult AB), November 1999.
IPR 00-22	Deconvolution of breakthrough curves from TRUE-1 tracer tests (STT-2) with sorbing tracers. Äspö Task Force, Task 4F. M Elert, H Svensson (Kemakta Konsult AB).

IPR 02-47 Complementary investigations at the TRUE-1 site. Crosshole interference, dilution and tracer tests, CX-1–CX-5.
P Andersson, E Wass, S Gröhn, M Holmqvist (Geosigma AB), May 2002.

SKB Technical Reports

TR-97-06 Äspö HRL – Geoscientific evaluation 1997/5. Models based on site characterization 1986–1995.
I Rhén (ed) (VBB Viak), G Gustafson (Chalmers University of Technology), R Stanfors, (RS Consulting), P Wikberg (SKB).

TR-99-04 Evaluation of modelling of the TRUE-1 radially converging and dipole tests with conservative tracers. Task 4C and 4D.
M Elert (Kemakta Konsult AB) May 1999.

TR-00-07 Final report of the first stage of the tracer retention understanding experiments.
A Winberg (Conterra AB), P Andersson (Geosigma AB), J Hermanson (Golder Grundteknik), J Byegård (Chalmers University of Technology), V Cvetkovic (Royal Institute of Technology), L Birgersson (Kemakta Konsult AB), March 2000.

TR-01-12 Evaluation of modelling of the TRUE-1 radially converging tests with sorbing tracers. Tasks 4E and 4F.
M Elert, H Svensson (Kemakta Konsult AB), May 2001.

TR-01-24 First TRUE Stage – Transport of solutes in an interpreted single fracture. Proceedings from the 4th International Seminar Äspö, september 9–11, 2000, SKB, 2001.

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