International
Progress Report

IPR-00-06

Äspö Hard Rock Laboratory

Test plan for

Groundwater flow modelling – natural barriers

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VBB-VIAK

December 1999

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Report no.	No.
IPR-00-06	F85K
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Approved	Date
Olle Olsson	2000-03-28

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Keywords: Groundwater flow modelling, natural barriers

Abstract

The Äspö Hard Rock Laboratory (Äspö HRL) is an essential part of the research, development, and demonstration work performed by SKB to with the purpose of designing, constructing, and licensing a final repository for spent nuclear fuel. The Operating Phase of the Äspö HRL will start in 1995 and is planned to extend to at least 2010.

Mathematical models for groundwater flow and transport are important tools in the work of waste disposal. SKB has during the years developed and tested a number of modelling tools and at Äspö HRL several modelling concepts as Stochastic Continuum (SC) and Discrete Fracture Network (DFN) concepts has been used. SC approach has been used for the regional and site scale models and in the laboratory scale model the starting point has been a fracture network for assigning hydraulic properties to a SC model. Based on the new data available since the Äspö model 1996, and the new concept of generating the conductivity field, it is planned to update the site, laboratory and (possibly) the regional models of Äspö area.

The first step is to further develop and test the concepts of the generation of the conductivity and porosity fields. The second step is to update the site, laboratory and (possibly) the regional models based on the new concepts and the updated geological and hydrogeological models of the Äspö site. Updating of the models of the Äspö site is made within the framework of a project called GEOMOD. Within the first (and possibly the second) step the methodology for calibration and conditioning, applying boundary conditions for tunnel system and importing and exporting data to/from RVS shall be further developed.

Contents

1 Background

The Äspö Hard Rock Laboratory (Äspö HRL) is an essential part of the research, development, and demonstration work performed by SKB with the purpose of designing, constructing, and licensing a final repository for spent nuclear fuel. The Operating Phase of the Äspö HRL will start in 1995 and is planned to extend to at least 2010.

The Äspö HRL is open to international participation to meet the needs of other organisations engaged in the disposal of radioactive waste. The Äspö HRL Project has so far attracted strong international interest and co-operative agreements have been signed with several organisations.

Mathematical models for groundwater flow and transport are important tools in the work of waste disposal. SKB has during the years developed and tested a number of modelling tools and at Äspö HRL several modelling concepts as Stochastic Continuum (SC) and Discrete Fracture Network (DFN) concepts has been used. SC approach has been used for the regional and site scale models (Svensson 1997a,b) and in the laboratory scale model the starting point has been a fracture network for assigning hydraulic properties to a SC model (Svensson, 1999b). The methodology of how to transform the fracture network to the SC was shown in Svensson (1999a). Based on the new data available since the Äspö model 1996, reported in Rhén et al (1997b), and the new concept of generating the conductivity field (Svensson,1999a), it is planned to update the site, laboratory and (possibly) the regional models of Äspö area.

Tests of embedded grids have been made with the PHOENICS code. The purpose was to see if it was feasible to generate local dense grids to get high resolution and better possibilities to define small features in the model. The technique is expected to be useful for regional, site and laboratory scale models. Both the non-uniform and BFC (Body Fitted Co-ordinates) grids generates cells with high aspect ratio, i.e. $\Delta_x/\Delta_y >>1$, which is a disadvantage when spatial assignment method for hydraulic conductivity is chosen. The advantage with embedded grid is that the cells are cubic which is considered better basis for choosing spatial assignment method. The test indicated that embedded grids might be feasible approach. However, it may (not) be a problem with the spatial assignment method in the BFC grid, with a limited aspect ratio, with the method for generating the hydraulic conductivity field mentioned below (start with a fracture network for calculation of the cell conductivities). It has however not been tested. At present the new technique is only adopted to handle BFC grids which are deformed in the vertical direction. In this way the topography can be handled in the same way as in Svensson (1997a,b)

2 Objectives

The general objective is to improve the numerical model in terms of flow and transport and to update the site-scale and laboratory scale models for the Äspö HRL. The models should cover scales from 1 to 10 000 metres and be developed for the Äspö site, but be generally applicable.

The objectives with the updated models are to:

- Test and improve new methodology of generating a conductivity field based on a fracture network in a continuum modelling approach.
- Develop models for transport and dispersion.
- Improve the methodology for calibration and conditioning the model to observed conductive features of the groundwater flow models.
- Improve the handling of the inner boundary conditions in terms of generating the tunnel system and applying boundary conditions.
- Improve the data handling in terms of importing geometrical data from RVS to the numerical code for groundwater flow and to export modelling results to RVS.
- Increase the details in the models based on new knowledge of the Äspö site collected during the last years.

The model code intended to be used is PHOENICS, which has been used in regional, site scale and laboratory models (Svensson 1997a,b and 1999b)

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3 Rationale

3.1 Relevance to repository performance, construction or licensing

Groundwater flow and transport modelling is important for the performance and safety assessments of a waste repository. Useful modelling tools must be available around 2001 at the time when the characterisation of two candidate repository sites will start.

Based on experiences from the safety analysis project SR 97 and international modelling projects within the Äspö Task Force (for example Gustafson and Ström (1995) and Gustafson et al (1997)) it has been found that both the concepts and the modelling tools should be improved to better fulfil the demands from the performance and safety analysis.

The present programme aim at developing the models to be feasible both for site description as well as for repository performance modelling.

3.2 Current state of knowledge

3.2.1 Groundwater flow modelling

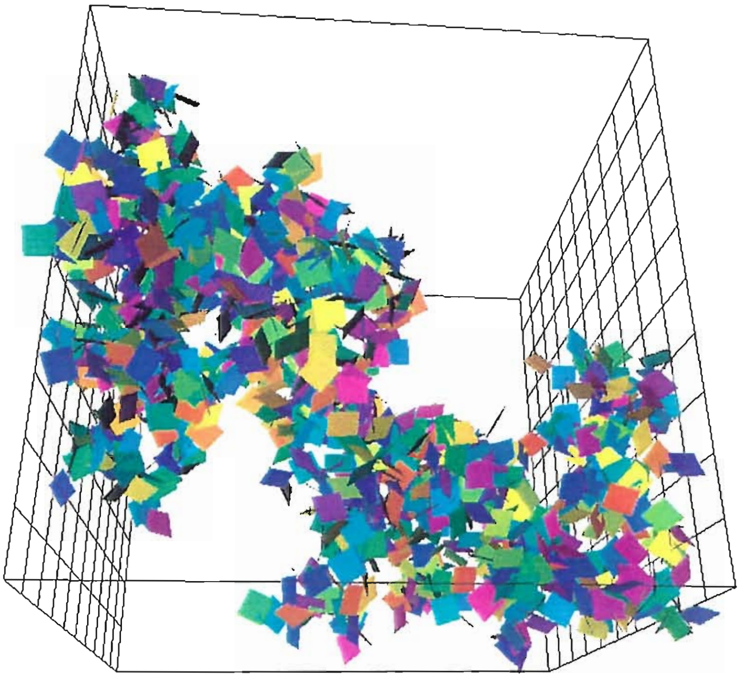
The modelling of groundwater flow and transport in sparsely fractured rock is made with three different concepts: Stochastic Continuum (SC), Discrete Fracture Network (DFN) and Channel Network (CN) The last modelling approach has similarities with the SC approach. Experiences gained from international modelling tasks within the Äspö Task Force on modelling of groundwater flow and transport of solutes have shown that the different concepts are all useful but there are needs to develop both the codes in terms of data handling and visualisation and to continue developing and testing the concepts (Gustafson and Ström, 1995 and Gustafson et al, 1997). The intention with this test plan is to develop the SC approach

The different modelling concepts have their benefits and drawbacks. It seems that SC approach may be most useful for the larger scales and the DFN approach have benefits in the smaller scale. The use of the SC approach demands that spatial correlation models can be established. The use of conventional geo-statistical methods has indicated problems when tests from borehole have been used. These methods do not take into account the support scale in proper manner and the long distances between bore holes are a problem when a 3D correlation structure is to be established ((La Point, 1994, La Point et al, 1995, Niemi, 1995, Walker et al, 1997). It was also stressed in Rhén et al

(1997a) the need to develop better spatial correlation models useful for the SC approach. One way of doing this is to incorporate geometrical models of the fracture network for the generation of the correlation model or directly create the conductivity field in a SC model. The first approach has been used by Hoech et al (1998) and the second approach has been used by Svensson (1999b). Important data for the test of the model in Svensson (1999b) is the statistics of hydraulic conductivity based on the injection tests made with 3 m packer spacing but also the statistics of the distances between conductive features exceeding a specified limit of the transmissivity. The last type of statistics was for Äspö data presented in Rhén et al(1997b) and later the analysis was updated with more data but focussed on High Permeability Features (HPF) (Rhén and Forsmak, 1999). Both the results from Hoech et al (1998) and Svensson (1999a,b) seem promising in terms of the possibilities of generation anisotropic conditions as well as a more realistic correlation structure in the SC models. In Figures 3-1 and 3-2 show two fracture networks at the percolation threshold when the network only connects two opposite faces of a flow domain modelled (Svensson ,1999a). A more advanced way of performing a geo-statistical analysis also indicate good correspondence between statistical model based on the injection tests made with 3 m packer spacing and the conductivity field in the laboratory model (Painter, 1999, Svensson, 1999b).

Transport properties was only briefly studied during the pre-investigation and construction phase of Äspö HRL. During the operation phase of the Äspö HRL much more effort are made to increase the knowledge of the transport properties in fracture crystalline rock. Some of the results concerning transport properties in fracture crystalline rock was compiled in Rhén et al (1997b) and was also used in the modelling (Svensson, 1997b). These relations are approximate and uncertain but still considered useful for assigning properties to the rock mass on a large scale. To some extent can these relations probably be updated with results from mainly the TRUE project (Winberg, (1996) and later reports from the project). Tests of modelling concepts for transport in SC have also been made. In Svensson (1992, 1994) it was tested how micro-dispersion and sorption could be incorporated into a particle tracking routine. It was further developed and tested in Svensson (1999c). The recent development in Svensson (1999c) is focused on description of physical and chemical processes. The basic idea in PARTRACK is that a particle can have two states "moving" or "non-moving". A frequency pair determines the rates by which a particle should change state. Obviously it is possible to describe sorption in this way but it has also been demonstrated that Taylor dispersion can be exactly parameterised by the two states. Up to now it has however not been possible to handle more than one process that causes dispersion. The recent development allows for several physical and chemical processes working in parallel. It is thus possible to simulate the movement of a particle that is exposed to, for example; Taylor dispersion when moving in the flow, diffusion into a stagnant pool, sorption on the walls of that pool and perhaps even diffusion into the rock matrix. The recent development of PARTRACK is employing some concepts and formulations from the Multi-rate model of diffusion (Haggerty and Gorelick (1995) and also the applications of McKenna (1999)) Presently the mathematical derivations, software development and some basic tests been carried out. It can be expected that future work should be directed to implementation of relevant physical and chemical processes.

In the site and regional models (Svensson, 1997a,b) the tunnel has been modelled as a line and the flow into the tunnel has been prescribed according to the measurements and distributed in the deterministic Hydraulic Conductor Domains. This has been considered to be a simple and straightforward technique and to give sufficiently good results in the regional and site scales. In the laboratory scale it is difficult to get a realistic pressure and flow field near the tunnels with the technique used for the site and regional scale models. The size of the tunnel, the smaller side tunnels or nisches should be modelled properly and a reasonable flow distribution along the tunnel must be given or generated by applying a pressure-boundary condition. It is difficult to define a distributed flow along the tunnel as the exact measurements are made ”only” every 150 m along the tunnel. There have been tunnel mapping of flowing feature that can be a base for defining a stochastic distribution but after that it still remains to find a way of applying it to the generate conductivity field around the tunnel. Probably a better way is to have a pressure boundary condition and try to define a generalised Skin factor that gives correspondence between the measured inflow to the tunnel and the generated conductivity field. This has been tested in the laboratory scale model but has to be improved. In the laboratory scale model it is also possible and useful to define minor conductive features close to the tunnels. Mapping and hydraulic tests along the tunnel, mostly at the experimental sites, give information of smaller conductive features that can be geometrically defined. If they are considered ”certain” it may be a reason to include them in the laboratory model. There is also information of where conductive features intersect longer core holes. This information is used to calculate the statistics of these features (See HPF below) and is very useful for the calibration of models. It can also be used to condition the model along the boreholes. It is how ever difficult because the orientation and size of the features are not always known and it is difficult to define an effective methodology for conditioning-calibration.



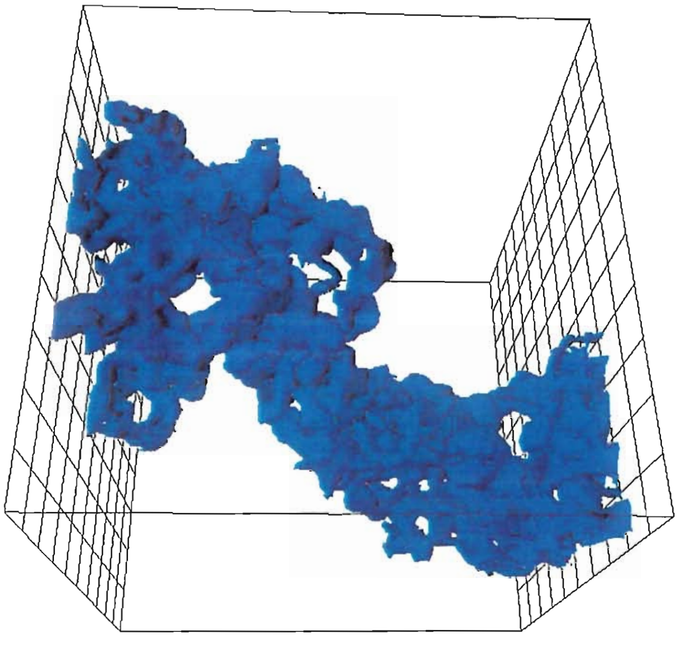


Figure 3-1. *A fracture network that connects two opposite faces of the box (top) and the corresponding flow channels. Fracture density at the percolation threshold. Fracture size is 5 m. The two connected sides of the box have been marked with grids.*

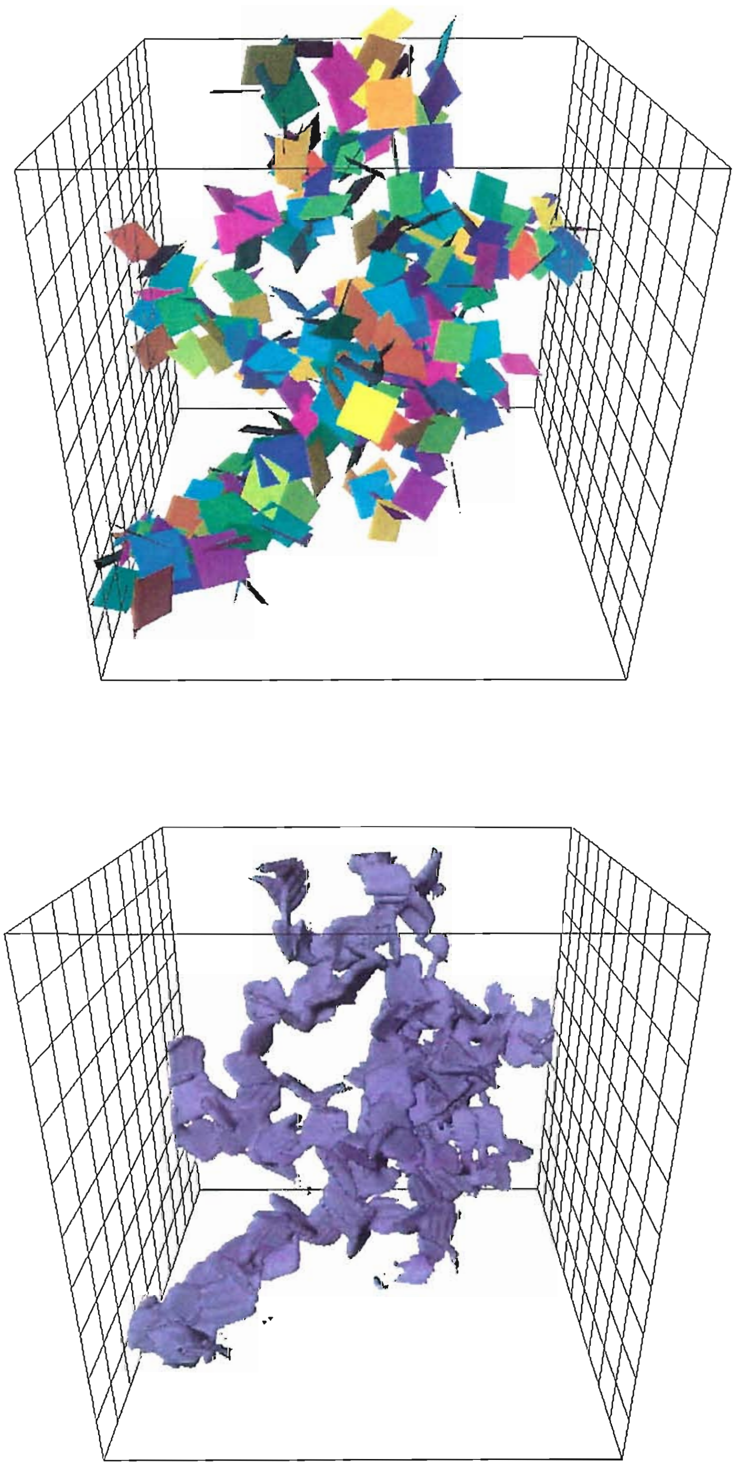


Figure 3-2. *A fracture network that connects two opposite faces of the box (top) and the corresponding flow channels. Fracture density at the percolation threshold. Fracture size is 10 m. The two connected sides of the box have been marked with grids.*

3.2.2 HPF, part 1

The results from the construction phase of the Äspö HRL showed a relatively high number of events with a high inflow rate during drilling. Features with a high transmissivity were drilled through a number of times and these features were in several cases not a part of the deterministically defined major discontinuities. This has also been seen during drillings in the operation phase of the Äspö HRL. It was therefore considered important to assess the possibility to predict fractures or features with high transmissvities from data collected during the pre-investigation phase.

A study was made of High Permeable Features at Äspö HRL (Rhén and Forsmak, 1999). With the term High Permeable Feature (HPF) it was understood a fracture, system of fractures or fracture zone with an inflow rate (observed during drilling or flow logging) which exceeds 100 l/min or alternatively show a transmissivity $T \geq 10^{-5}$ m^2/s.

The objective of the study was to:

- Compile information that can be coupled to High Permeable Features at southern Äspö.
- Analyse these data statistically and investigate possible correlations between HPF and other observed features.

It was of interest to make a first attempt at setting the occurrence of HPFs in a structural geological context. Of special interest in this study is shown if HPFs occurs in the vicinity of :

- any special rock type
- any special rock contact
- rock veins
- crush zones/natural joints
- areas where RQD is high/low

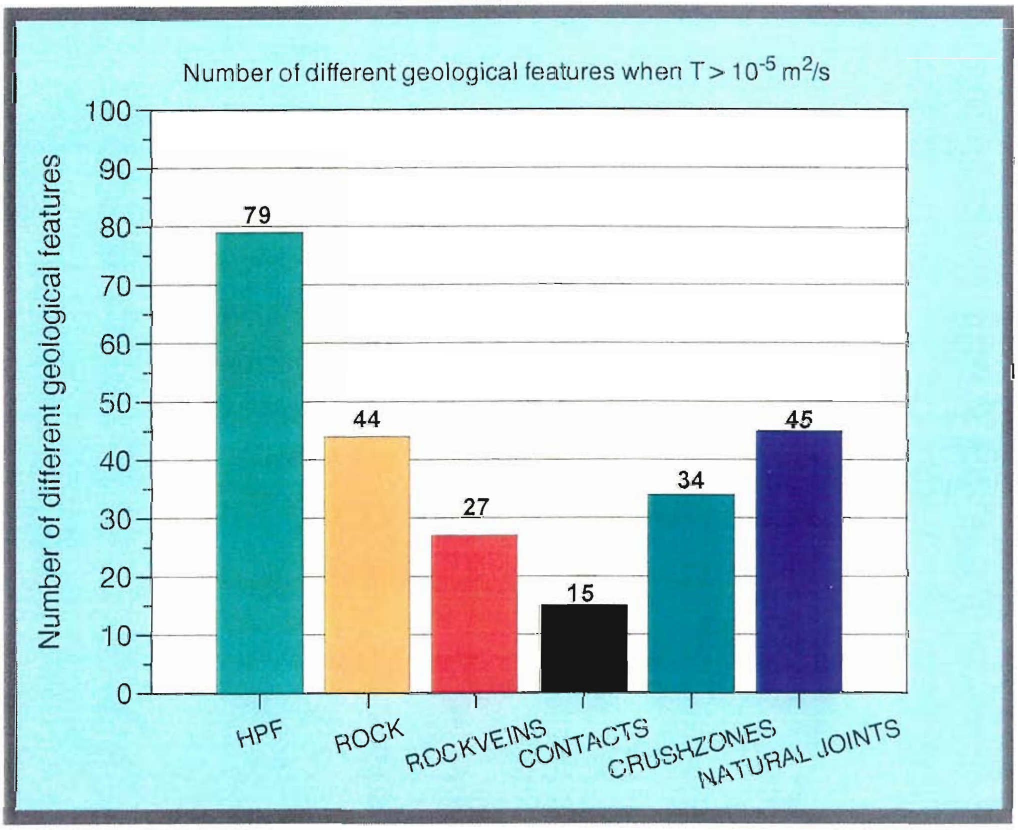
The evaluation of HPF:s for the surface bore holes is based on the injection tests with a packer spacing of 3 metres and accordingly the geological data for the same packer interval.

The evaluation of HPF:s in the tunnel core holes is based on positions of flows into the bore holes. If these are based on drilling records it is judged that there exist an uncertainty of +/- 1-meter from the given position. If flow logging is the basis of position it is judged as more certain. However, in this evaluation +/- 1 meter from the observed HPF has been the basis for the bore hole section to be used for the evaluation.

In the bore holes mentioned above the total number of HPF:s, based on $T \geq 10^{-5}$ m^2/s are 79, and the correlation study is based on those data.

The results of the correlation study are presented in *Figure 3-3.* A total of 79 HPF:s were identified in the bore holes studied. In those cases where a HPF occurs there must be a crush zone or a natural joint. Of these 79 cases, 34 were related to a crush zone while in 45 cases there was one or several natural joints in the section defined for the HPF.

There are normally just one rock type (not taking into account the veins) within the interval for the HPF:s. Rock veins are found in 27 sections and rock contacts are found in 15 sections, and among these, rock veins and rock contacts are both found in 7 sections. If sections having veins or rock contacts are excluded, still 44 sections of 79 have just one rock type, see *Figure 3-3.* In 15 of these 44 sections, the rock type is fine-grained granite. In 37 of the 79 sections, fine-grained granite is present, if sections with veins of fine-grained granite are also included.



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CRITERIA :

TUNNEL BOREHOLES - HPF POSITION +/- 1 meter
SURFACE BOREHOLES - WITHIN PACKER INTERVAL (3 m)

Figure 3-3. *The total number of HPF:s and the number of different geological features within an interval associated to the HPF.*

The definition of the HPF:s (High-Permeability Features) as having a transmissivity $T \geq 10^{-5}$ m^2/s or a flow rate $Q \geq 100$ l/min into a bore hole with pressure close to atmospheric was more or less arbitrarily chosen for this study. However, it was known from the previous studies at Äspö HRL that features, with properties around these values mentioned above, were not uncommon and not all of them could be explained by fracture zones with large extent defined deterministically using geological, geophysical, hydrogeological and hydrochemistry data. This study has shown this in a more clear way and the main conclusions are presented below.

HPF:s and large deterministically defined fracture zones:

- About 50 % of the HPF:s can be connected to the deterministically defined fracture zones with a large extent, which were based on evaluation of geological, geophysical hydrogeological and hydrochemistry data. The rest of the HPF should be modelled as fairly large features in-between the deterministic zones. The radius of these features may be around 30-100m.
- The implication of the size of the HPF:s is that there should be a correlation model for assigning hydraulic properties to the hydraulic rock domains taking the size into account. The present SKB model of Äspö from 1997 does not consider this. The hydraulic conductor domains in the present model are not affected by the present results.

Distances between HPF:s:

- The distances between HPF:s have a lognormal distribution.
- The arithmetic mean distance between HPF:s, defined as features having a transmissivity $T \geq 10^{-5}$ m^2/s, is for the sub-vertical bore holes drilled from surface 75–106 m. The arithmetic mean distance between HPF:s, is for the sub-horizontal bore holes drilled from the tunnel spiral 73-106 m. The corresponding geometric mean values are 24-27 m and 27 - 34 m respectively. Possibly, the distances estimated from the sub-vertical boreholes should be somewhat larger than the figures given above.
- The statistics of the distances is dependent of the scale of observations. It is possibly better to use larger interval than 3 m to describe the spatial distribution of distances between HPF:s on a scale of several hundred meters, at least if simple measures as arithmetic mean is used as a measure for HPF:s between the large deterministic zones.

The coupling between HPF and lithology and fracturing:

- Somewhat less than half of the HPF:s can be explained by what was classified as crush zones during the mapping of the cores and the rest by one or a few natural joints. It clearly shows that high permeability features exist in the sparsely fractured rock mass. The evaluation of the RQD for the intervals having a HPF shows the same thing, both very low and very high RQD value are found in the bore hole intervals having a HPF.
- HPF:s are most frequent in fine-grained granite, taking into account the amount of different rock types at Äspö HRL. Äspö diorite and Småland (Ävrö) granite, which are the dominating lithological units, have approximately the same frequency of HPF:s and is about half of the frequency in fine-grained granite. The frequency of HPF:s in greenstone is somewhat greater than in Äspö diorite and

Småland (Ävrö) granite. In pegmatite and mylonite-hybridized rock the frequency is about the same as in greenstone, but the conclusion is very uncertain due to the small sample size

- Only about 20 % of the HPF:s are found near rock contacts. Fine-grained granite is the dominating rock type found in these rock contacts.

4 Scope

4.1 Project tasks

The main tasks are:

- Feasibility project A, Flow modelling
- Feasibility project B, Transport
- HPF, part 2
- Update the regional scale model
- Update the site model
- Update the laboratory model

The two first tasks aims at developing and testing the numerical code for the flow and transport calculations, which is made before the models are updated. The third task aims at compiling some site-specific data useful for the updating of the models. Useful data for the updating of the models is also supported by the GEOMOD project, which is described in Section 4.2. The three first tasks are the basis for the three last tasks. Below the tasks are described in more detail.

Feasibility project A, Flow modelling

Objective: Evaluate and test the main new features of the flow model. It is not necessary to deal with calibration or realistic boundary conditions

The following topics are included:

- GEHYCO concept development. The flow paths and the stagnant pools in a fracture net work are dependent of the connectivity of the fractures and the density distribution in space and time of the water. Concepts of the connectivity, total porosity and flow porosity and how it is included in the SC model should be made and tested. A number of test cases should be made to get a better understanding of the flow paths and transport and how it is related to the concepts used and the application of the numerical model. The influence of the cell size for flow through a block or towards a bore hole section are examples of such studies.
- GEHYCO concept development. " Which fractures should be deterministic on a certain model scale?" Test the flow capacity and distribution of pressure and salinity on the boundaries of a block with different cell sizes and lower limit for fracture sizes. The purpose is to see when and how the background conductivity (a minimum value for each cell independent of the fracture transmissivities or dependent of the cell size and the fractures not included in the cell wall conductivities) should be modified in order to preserve the flow capacity of the block, which should be correlated to cell size and the minimum sizes of the fractures included. The

distribution of pressures and salinity on the boundaries is of interest when these properties are to be transferred to another model. It is of interest to see how the variability of pressures and salinity on the boundaries changes with cell size and minimum sizes of the fractures included.

- GEHYCO concept development. Update the model for correlation between fracture aperture and transmissivity and calculate the effective porosity. Include the probable numbers of fractures based on the transmissivity and calculate the fracture surface area. The numbers of fracture are simulated as a specified function of transmissivity or with a probability function that is dependent of the transmissivity. Relation are taken from Rhén et al (1997b) or updated relations.
- Embedded grid technique in Cartesian grid. Total number of cells that are feasible should be tested.
- Describe topography in a Cartesian grid. Test how much is the computer time decreased and test how well the streams and soil cover be simulated compared to BFC (Body Fitted Co-ordinates) net
- Alternatives to simulate the tunnels. For regional scale it is probably best to prescribe the inflow, but on the smaller scales a fixed pressure boundary condition with skin is preferred. The methodology of how to effectively apply fixed pressure boundary condition with skin to a tunnel should be developed. Total infow to a tunnel section, distribution of mapped flow rates and distribution of minor features intersecting the tunnel can be a basis for calibration routines.
- Include CAD-files from RVS. Import tunnel geometry from RVS and create routines for defining the Finite Volume net and pressure boundary conditions

Feasibility project A will probably be divided into three parts: development of the GEHYCO concept, development of gridding technique and boundary conditions for tunnels and finally, testing data exchange with RVS.

Feasibility project B, Transport

Objective. Demonstrate the possibilities to simulate transport in the model created according to GEHYCO using PARTRACK and Fluid Population Method for the transport simulations. The transport is studied from smaller to larger scales:

- Single fracture
- Fracture zone
- A block
- Site scale

Last two parts are possibly integrated in one modelling task. It is expected that the new version of PARTRACK will be a useful tool for simulating transport and dispersion (sorbing and non-sorbing tracers). Initially the development will be focus on:

- Evaluate if the multi-rate model by Roy Haggerty can be used as a sub-grid model in PARTRACK.
- Simulate a suitable experiment from Task 4.

- Understanding processes.

Feasibility project B will probably be divided into three modelling parts; single fracture model, fracture zone model and block and site scale model.

HPF, part 2

It is planned to update some of the results in Rhén and Forsmark (1999), mainly the distance statistics for conductive features. There are now available more data from new bore holes that are useful for updating of the statistics of the HPFs, and more important, to calculate the distance-statistics for features with transmissivies that are lower than the one defined for the HPF:s in Rhén and Forsmark (1999).

Updating of the regional scale model, the site model and laboratory model

The updating of the models is performed as three tasks:
- Update the regional scale model
- Update the site model
- Update the laboratory model

However, if embedded grid technique is successful, the three models to be updated may formulate as follows:
- Regional/Site model
- Site/Laboratory model
- Laboratory/ Experimental model

The reason for considering two scales at the same time is that consistency of flux over boundaries can then be assured through the embedded grid technique. Each model will be based on the following steps:

- Update the structural model of the deterministic Hydraulic Conductor Domains (HCD) based on GEOMOD

- Update the spatial model for the fracture geometry (spatial distribution of centre of fracture, fracture size and fracture orientation) results from Prototype Repository and possibly other projects.

- Update the model for correlation between fracture size etc and transmissivity

- Test and calibrate the models based on hydraulic tests (LPT2, tunnel draw-down etc) and statistics of results from hydraulic tests as for example HPF:s (see below)

4.2 Supporting project tasks

4.2.1 GEOMOD

In Rhén et al (1997b) models of geology, mechanical stability, hydrogeology, hydrochemistry and transport of solutes was presented. These models were the basis for the previous groundwater flow models (Svensson 1997a,b, 1999b). New data are now available and a project called GEOMOD has started that aim at updating the models of the deepest part of the Äspö tunnel. From hydrogeological point of view it is expected that for example a number of new minor conductive features (zones) along the tunnel will be defined deterministically in space.

4.3 Time schedule

The entire project duration is four years 1999 included. Feasibility project A, Flow modelling, Feasibility project B, Transport and HPF, part 2 is planned to be made during year 2000. Feasibility project A starts early 2000 and continues probably to late 2000. Feasibility project B and HPF part 2 starts spring or summer 2000 continues to late 2000. Updating of the regional scale model and the site model is planned to be made during year 2001. The laboratory model is planned to be made early year 2002.

The supporting project GEOMOD is planned to start summer 1999 and reported late 2000.

5 Project organisation and resource requirements

5.1 Organisation

The project manager is Ingvar Rhén, VBB-VIAK. Urban Svensson CFE performs model development and the updating of the models.

Delivery of data to and from SICADA and RVS is made by Ebbe Ericsson at Äspö HRL .

VBB VIAK performs HPF study.

5.2 Data management

Delivery of data to and from SICADA and RVS are reported in log files that are included in the appendices of the report(s).

5.3 Reporting

Model development is presented as Progress Reports (IPR). The updated models are presented in Technical Report(s) (TR). The report(s) is (are) also made in a digital format that is sent to SKB

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