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Natural Barriers – Summary of results from experiments at Äspö HRL and related analysis performed 1995–2000

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Foreword

This report has been compiled by a group consisting of the principal investigators and project managers of experiments and projects related to the function of the natural barrier*) primarily performed at the Äspö HRL.

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*) The bedrock with available fractures and fracture zones, its properties and on-going physical and chemical processes which affect the integrity of the engineered barriers and the transport of radionuclides.

Abstract

The barrier functions of the bedrock, with respect to the safety of a nuclear waste repository, can be divided into isolation, retention and dilution. Experiments carried out at the Äspö Hard Rock Laboratory aim at increased knowledge of these functions, and thus to reduce the uncertainty in the safety assessment.

This report describes the purpose, objectives and major achievements of those experiments, which have been conducted during 1995–2000. The experiments are within the disciplines of hydrogeology, hydrochemistry, geochemistry and geology.

Sammanfattning

Bergets säkerhetsmässiga barriärfunktioner kan uppdelas i isolering, fördröjning och utspädning. Experiment som syftar till att öka kunskapen om dessa barriärfunktioner och därigenom minska osäkerheterna vid analys av djupförvarets långsiktiga säkerhet pågår vid Äspölaboratoriet.

Rapporten beskriver experiment som utförts under perioden 1995–2000. Deras syfte och väsentligaste resultat samt i förekommande fall kvarstående frågor belyses. Beskrivna experiment berör hydrogeologi, hydrokemi, geokemi och geologi.

Contents

1 Introduction

1.1 The Äspö Hard Rock Laboratory

The Äspö Hard Rock Laboratory constitutes an important component of SKB's work to design, construct, and implement a deep geological repository for spent nuclear fuel and to develop and test methods for characterisation of selected potential repository sites. In the autumn of 1986, SKB initiated field work with the objective to site an underground laboratory in the Simpevarp area in the municipality of Oskarshamn. Construction of the Äspö Hard Rock Laboratory started on October 1st, 1990, after approval had been obtained from the authorities concerned. Excavation work was completed in February 1995.

The Äspö Hard Rock Laboratory has been designed to meet the needs of the research, development, and demonstration projects that are planned for the Operating Phase that started in 1995. The underground part of the laboratory consists of an access tunnel from the Simpevarp peninsula to the southern part of Äspö where the tunnel continues in a spiral down to a depth of 450 m.

1.2 The safety function of the hostrock

Tests of models for groundwater flow, radionuclide migration and chemical/microbial processes are one of the main purposes of the Äspö Laboratory. The rock surrounding the repository constitutes a natural barrier to release of radionuclides from a deep repository. The most important function of the natural barrier is to provide protection for the engineered barriers through stable chemical and mechanical conditions and to limit transport of corrodants and radionuclides through slow and stable groundwater flux through the repository and reactions of radionuclides with the host rock. The programme includes projects with the aim to evaluate the usefulness and reliability of different models and to develop and test methods for determination of parameters required as input to the models.

The barrier functions considered when assessing the long-term safety of a deep geological repository are *isolation, retention* and *dilution*. These functions are provided by the very existence of the bedrock, its properties and the on-going processes in the rock. The goal of the experiments within Natural Barriers is to increase understanding of these processes and to increase the scientific knowledge of the safety margins of the deep repository and to provide data for performance and safety assessment calculations. The priority for the on-going experiments on the natural barriers is to concentrate the efforts on those experiments which results are needed for the planning of the site investigations, planned to start in 2002.

Isolation is the prime function of the repository. It is obtained through the co-function of the engineered and the natural barriers. In the KBS-3 disposal concept the copper canister is expected to remain unbroken for millions of years, in case it is intact at deposition. The bentonite clay barrier will further protect the copper canister by minimising the flow of water to the canister and thereby minimising the transport of possible corrodants to the canister. For other waste types, not insulated by copper, the flow of water to the canister/waste containment is largely determining the magnitude at which the corrosion and the dissolution of the waste form can take place. For a good isolation it is thus necessary to minimise the groundwater flow to the waste containment.

Additional conditions that affect the isolation are the chemistry of the groundwater and the mechanical stability of the rock. Present day hydrochemistry including reducing conditions is favourable for a low corrosion rate of the canister. These conditions can be expected to persist up to, at least, the next major glaciation. The host rock should provide mechanical protection for the engineered barriers and future rock movements should not jeopardise the integrity of the engineered barriers. This can be achieved by proper repository design and emplacement of spent fuel away from active faults.

Conceptual and numerical groundwater flow models have been developed throughout the Äspö project. Further development of the tools for groundwater flow and transport calculations is made to meet the needs of the site characterisation phase.

Hydrochemical stability has been assessed for both present day as well as previous conditions. The aim has been to explain possible chemical conditions in a repository host rock based on assumption of different climate conditions in the future. On-going projects aim at investigating the chemistry of the water in the pores of the rock matrix, and to better understand the microbial effects on groundwater chemistry.

The *retention* of radionuclides dissolved in groundwater is the second most important barrier function of the repository. Retention will be provided by any system and process that interacts with the nuclides dissolved in the groundwater when eventually the water has come in contact with the waste form and dissolved radionuclides. Retention is provided by the physical and chemical processes, which occur in the near field and far field. Some elements are strongly retarded while the non-sorbing nuclides are migrating with the speed of the flowing groundwater. The major emphasis in the safety assessment calculations has been on the weakly retarded nuclides because these can potentially be transported up to the biosphere.

No specific experiment is focussing on dilution.

1.3 Purpose of this report

The purpose of this report is to give a Summary of the Results obtained within the programme Natural Barriers during the period 1995–2000. The projects/experiments are reported one by one without any synthesis.

2 Reported experiments related to Natural Barriers

Transport and retention of radionuclides have been investigated *in situ* and in the laboratory in the TRUE-1 and TRUE Block Scale projects. Conceptual and numerical modelling of groundwater flow were studied in the Fracture Characterisation and Classification (FCC) and in the High Permeability Features (HPF) projects.

Experiments with strongly sorbing radionuclides are carried out in the CHEMLAB probes within the RadioNuclide Retention (RNR) projects.

Redox conditions have been investigated in the REX experiments.

Hydrochemical Stability, EQUIP and Matrix Fluid Chemistry deal with the hydrochemical conditions in a repository lifetime perspective. TASK#5 integrates the hydrogeological and hydrochemical data into numerical models describing the dynamic groundwater situation during the excavation of the Äspö tunnel.

Degassing and Two Phase Flow projects consider these aspects in the Äspö groundwater conditions.

Table 2-1 lists the safety functions assessed by the different projects and the major scientific investigation area(s).

Table 2-1. The reported projects and their barrier function.

Project	**Barrier Function (discipline)**
TRUE (Tracer Retention experiments)	Retention (Hydrogeology, hydrochemistry)
FCC (Fracture Characterisation and Classification)	Retention (Geology, geochemistry, hydrology)
HPF (High Permeability Features)	Isolation (Hydrogeology, geology)
RNR (Radionuclide Retention experiments in CHEMLAB)	Retention (Hydrochemistry)
REX (Redox Experient in detailed scale)	Isolation (Hydrochemistry, geochemistry)
Hydrochemical Stability	Isolation (Hydrochemistry)
EQUIP	Isolation (Hydrochemistry, geochemistry)
Task #5	Isolation (Hydrogeology, hydrochemistry)
Matrix Fluid Chemistry	Retention (Hydrochemistry)
Degassing-Two Phase Flow	Retention (Hydrogeology)

3 Tracer Retention Understanding Experiments TRUE

In order to obtain a better understanding of radionuclide transport and retention in fractured rock and to increase confidence that the radionuclide transport models intended for use in the licensing of a deep repository for spent fuel are based on realistic assumptions, a program has been devised for carrying out *in situ* tracer tests on different length scales. The program has been given the name Tracer Retention Understanding Experiments (TRUE). The overall objectives of the program are to increase the understanding of radionuclide transport and retention in fractured rock; further to show that utilised model concepts are based on realistic descriptions of fractured rock, and to investigate whether relevant input data for model parameters can be obtained from site characterisation, and finally to collect *in situ* data on radionuclide retention at different length scales. The experimental program is designed to generate data for conceptual and numerical modelling at regular intervals. Regular evaluation and review of test results will provide a basis for planning of subsequent test cycles. This should ensure a close integration between experimental and modelling work.

3.1 TRUE-1 experiment

3.1.1 Purpose and objectives

The First TRUE Stage (TRUE-1) was conducted with the objective to study transport and retention of sorbing radiotracers in an interpreted single fracture in the detailed scale (L<10 m). Specific objectives with the experiments were to investigate the experimental site with non-sorbing (conservative) and sorbing tracers in simple test geometry. Further to show that available tracer test technology could be transferred to ambient Äspö HRL conditions featured by high hydraulic pressure and high salinity of the groundwater at approximately 400 m depth. Secondary objectives included development and test of methods for assessing the pore space of the investigated fracture system using injection of epoxy resin, followed by excavation and analysis.

The TRUE-1 tracer tests were performed over distances of ranging from 3–10 m in the interpreted Feature A. Tests with radioactive sorbing tracers were performed in two source-sink pairs at a distance of about 5 m, employing radially converging test geometry.

3.1.2 Major achievements and conclusions

The TRUE-1 experiment has now been completed and the final has been prepared. The main conclusions from the First TRUE Stage (TRUE-1) are /Winberg et al, 2000/:

- Available tracer test methodology has been successfully been adapted and applied in the detailed scale at prevailing conditions (high hydraulic pressures (P >30 bars) and high salinity ([Cl] > 5000 mg/l).

- Sorbing tracers featured by sorption by cation exchange have been successfully applied in laboratory experiments and in *in situ* experiments.

- Breakthrough in the *in situ* experiments has been observed for the sorbing tracers Na^+, Ca^{2+}, Sr^{2+}, Rb^+, Ba^{2+}, Cs^+, K^+ and Co^{2+}. Uranine, tritiated water (HTO), $^{131}I^-$ and $^{82}Br^-$ were in this context used as conservative tracers.

- The sorptivity of the tracers used in the laboratory experiments on geological material from Äspö, show the following relative order; $Na^+ < Ca^{2+} \approx Sr^{2+} << Rb^+ \approx Ba^{2+} < Cs^+$. The observed relationship is also consistently observed in the *in situ* test results.

- The developed Lagrangian evaluation framework (LaSAR) /Cvetkovic et al, 2000/ has been found suitable for modelling the dominant effects of reactive transport in an interpreted single fracture.

- The evaluation identifies unlimited diffusion/sorption in the rock matrix as the dominant retention mechanism in Feature A over the time scales of the *in situ* experiments, particularly so for the more strongly sorbing tracers, e.g. Cs. The effects of equilibrium surface sorption, limited sorption in (fine-grained) gouge material and diffusion into stagnant zones are not found to be important for strongly sorbing tracers.

- The parameter values for diffusion/sorption estimated for *in situ* conditions have been shown to be enhanced compared to those measured in the laboratory on intact generic bedrock material. Diffusion/sorption enhanced with a factor f = 33–50 (excluding Cs) and f=137 for Cs has been evaluated for the different sorbing tracers and experiments. The enhancement is mainly attributed to increased matrix porosity and/or diffusivity, and matrix sorption applicable to *in situ* conditions, particularly in the altered rim zone of the fracture.

- Over time scales relevant to performance assessment, the role of altered rim zone of fractures is assumed to be second order, relative to that provided by the intact rock matrix.

- The processes identified in the TRUE-1 experiments and their relative importance, identified at the experimental time scales, are assumed valid also for Performance Assessment time scales. Laboratory data on unaltered intact rock, not associated with fracture rim zones, are assumed applicable over performance assessment time scales.

- A workable technology and procedure for obtaining pore space/aperture data from *in situ* epoxy resin injection and subsequent excavation and analysis has been developed and tested in a Pilot Resin Injection Experiment (performed in a network of less transmissive fractures compared to Feature A located in the F-tunnel adjacent to the lower shaft station).

The results from the TRUE-1 experiments also include an *in situ* demonstration of strong retention of Cs in crystalline bedrock. These findings coincide with the laboratory based indication that Cs exhibits slow reversibility in sorption, or even irreversible sorption. At the time of discontinuation of the TRUE-1 tests with sorbing tracers, the total recovery of Cs is about 40% after some 11000 hours (15 month) of pumping, implying that approximately 60% is sorbed in the injection section and in the fracture.

3.1.3 Remaining questions

The TRUE-1 experiments have been subject to scoping calculations, predictions and evaluation using a variety of different modelling concepts/approaches /Elert, 1999; Elert and Svensson, 2001/. The performed analysis show that the experimental results may be explained with alternative conceptual models, e.g. models which accounts for more pronounced heterogeneity and subdivision into multiple flow paths combined with an assumed presence of high porosity fine-grained fault gouge /Mazurek and Jacob, 2001/. Similarly, the noted enhanced diffusion/sorption can alternatively be explained by transport experiencing more flow-wetted surface area through a more pronounced three-dimensional flow pattern /Neretnieks and Moreno, (in prep.)/. An international seminar focused on the results of the First TRUE Stage and the role of *in situ* tracer experiments in site characterisation was held in September 2000 /SKB, 2001/. It was here recommended that complementary field work should be performed at the TRUE-1 site in order to improve understanding of the three-dimensional fracture network to which Feature A is connected. Further, to carry out complementary tracer dilution experiments and tracer tests employing alternate sinks to further improve the three-dimensional understanding of the investigated site prior to the planned resin injection, the latter which will be carried out 2004/2005. The reason for this postponement is activities in the neighbouring LTDE experiment, see below.

The Long-Term Diffusion Experiment (LTDE) /Byegård et al, 1999/ is intended as a complement to the dynamic *in situ* experiments and laboratory experiments performed in the TRUE Programme. The background being the fact that any diffusivity measurements conducted on core samples from deep seated bedrock will be affected by relief of rock stresses which may result in elevated porosity and diffusivity compared to that of the intact unfractured bedrock *in situ*. The basic idea of the experiment is to locate a static tracer experiment to an unfractured rock mass with the intention to characterise diffusion of radionuclides into the rock matrix. The experimental concept is based on a large diameter borehole that exposes a natural fracture surface (core stub) that is packed off with a cap. Performed scoping calculations using available diffusivity data indicates that axial diffusion will range from millimetres for the strongly sorbing tracers to decimetres for the weakly sorbing tracers considered. A suitable target fracture has been identified in borehole KA3065A02 about 10 m from the tunnel. During 2000 a telescoped experimental borehole (300/196.5 mm) was drilled with the intention to leave a core stub in the borehole with a diameter of 177 mm and a length of 50 mm. Unfortunately, the core stub turned out to be 150 mm, i.e. three times as longer than originally planned. This called for revisit of the geological and rock mechanical premises for the planned experiment. The outcome being that a modified experimental concept was devised where the study of sorption dominated aspects are retained in association with the exposed fracture surface. However, in order to reach intact rock a slim (36 mm) borehole will be drilled through the core stub and about a metre beyond. Through a specially devised injection scheme both axial diffusion into the core stub as well as radial diffusion from a section of intact rock in the slim hole will be possible.

An important component of the experiment is the construction of a downhole borehole equipment made up of mechanical and hydraulic packers and a regulation and sampling equipment which will be hosted at the borehole collar.

The duration of the circulation of traced groundwater is expected to be in the range of 3–4 years after which the telescoped borehole will be continued pass the rock volume of interest (overcoring) upon which analysis of the extracted rock volume for tracer activity will follow.

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3.2 TRUE Block Scale

3.2.1 Purpose and objectives

In the TRUE Block Scale /Winberg, 1997/, the experiences from the First TRUE Stage have been transferred and tested over larger length scales, and somewhat longer transport times. The specific objectives of TRUE Block Scale are to increase the understanding of transport and retention in a network of fractures/structures over a length scale of L=10–100 m. Further, to increase the ability to carry out predictions of transport and retention at the length scale considered. In addition, to study the relative importance of the retention processes (sorption and diffusion) and available pore spaces for diffusion, and finally to explore the possibility to use hydraulic data for transport predictions. A key issue is whether the exposure to a higher degree of heterogeneity experienced in the block scale will result in a higher degree of retention compared to that seen in the detailed scale TRUE-1 experiments.

The TRUE Block Scale Experiment is undertaken as a joint project between ANDRA, Enresa, JNC, Nirex, Posiva, and SKB. The total duration of the project is approximately 5.5 years with a scheduled finish at the end of the year 2001.

The project has been performed in a series of stages starting with scoping work and preliminary and detailed characterisation. In total six boreholes have been drilled into the experimental volume located at the 450 m level from two different elevations in the laboratory, all equipped with multi-packer systems consisting of 5–10 sections. The experimental array has been successively developed in an interactive fashion with a strong element of interactivity between site characterisation and modelling.

3.2.2 Major achievements

The interactive approach which provided the drive to the characterisation, and defined the need for additional boreholes, have helped to produce a relatively robust hydrostructural model of the investigated site including some 24 deterministic structures. A subset of those has been used in the subsequent block scale tracer tests. Fractures, which have not been attributed to deterministic structures, have been referred to a background fracture population described by specified statistics. The principal tools used when building the hydrostructural model have been borehole TV imaging (BIPS), Posiva DIFF flow logging (identification and quantification of conductive structures) and hydraulic pressure responses obtained from drilling and from cross-hole interference tests (hydraulic connectivity). It has further been identified as crucial to jointly merge and integrate geological and hydraulic information simultaneously to expedite construction of a realistic hydrostructural model.

Subsequently performed tracer dilution tests performed at ambient and pumped conditions have been used to verify the hydrostructural model and further to identify suitable borehole sections for injection of tracers. Midway in the project preliminary tracer tests were successfully conducted which demonstrated the feasibility of carrying out tracer tests in the block scale /Winberg, 2000/. The Tracer Test Stage have included a series of test phases where a) the basis was established for selecting a suitable sink section for subsequent tests with radioactive sorbing tracers, b) a satisfactorily high tracer mass recovery was demonstrated (> 80%) for the conservative species, which qualified a given source-sink set-up for usage of sorbing tracers, and finally c) a series of four injections with radioactive sorbing tracers were conducted in three source-sink pairs.

During the course of the project five different modelling concepts have been utilised. These include stochastic continuum, discrete feature network, and channel network models. In addition the LaSAR concept extended to the block scale and the so-called POSIVA concept have been used. A selection of the tracer experiments, including the tests with sorbing tracers has been subject to prediction and evaluation using the developed numerical models.

Presently the TRUE Block Scale Project is in the process of being reported in a series of four final reports.

3.2.3 Remaining questions

It is envisaged that there will be remaining issues following completion of the presently ongoing TRUE Block Scale Project. In addition, the available borehole array facilitates additional tracer test set-ups. To harbour these prospects a separate project has been divided, denoted TRUE Continuation, which contain a modelling part (BS2A) and a *in situ* tracer test and evaluation part (BS2B). The former will be used to formulate hypotheses that can be addressed by the subsequent *in situ* test phase. A third component is the planned complementary work to be performed at the TRUE-1 site, cf. Section 3.1.3.

3.2.4 References

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4 FCC – Fracture Characterisation and Classification

4.1 Purpose and objectives

The objectives of the Fracture Classification and Characterisation Project (FCC), a joint undertaking of Nagra (Switzerland) and SKB (Sweden), are:

- to classify water-conducting features occurring in the Äspö tunnel system
- to characterise and conceptualise these features with respect to radionuclide transport properties (e.g. structure, mineralogy, distribution of flow and matrix porosity)
- to develop and apply a methodology for the characterisation of water-conducting features in crystalline rocks.

The investigation methodology involves a stepwise procedure:

- Compilation of an inventory of existing data (geology, hydrogeology, hydrochemistry) and of the boundary conditions for exploration of water-conducting features (e.g. in boreholes, open tunnel). Definition of the scale which the investigation should target.
- Preliminary characterisation of a limited number of typical water-conducting features, with the objective of understanding the processes governing the evolution of water-conducting features and thus defining a set of geological parameters that adequately describe the features.
- Full characterisation of a large number of water-conducting features and development of a database containing all relevant parameters that can be observed or measured.
- Database analysis (which parameters are common to all features, which vary systhematically?) and derivation of a fracture classification scheme.
- Derivation of simplified conceptual models of all types of water-conducting features, including geometric and lithological (mineralogical, porosity) information required for transport modelling.
- Transport modelling and sensitivity analysis of parameters from the conceptual models.

The preliminary characterisation stage indicated that, on an observation scale of metres to decametres, all water-conducting features are related to faults.

4.2 Major achievements

Fault geometries and other parameters are indistinguishable between the Småland Granite and the Äspö Diorite. Fracture frequencies are higher in the Fine-grained Granite, and other fault characteristics contributing to transport properties (e.g. lithology, mineralogy, pore-space distribution) are also different. However, Fine-grained Granite was never observed to be the dominant host rock of any of the features because it occurs as small intrusive bodies or dykes measuring several metres to a few decametres in size. It is concluded that, because (within the database of 88 water-conducting features) this rock type does not host faults over more than a few metres, it is not relevant for the larger-scale transport properties of the faults.

The only striking difference between individual water-conducting features is the internal fault geometry; no other distinguishing criteria (such as the arrangement of lithological domains, mineralogy of fracture infills, transmissivity, etc.) were identified and probably do not exist. On the basis of the geometric arrangement of master faults and splay cracks in faults, 5 types of water-conducting features are distinguished:

- Type 1 – single fault
- Type 2 – swarm of single faults
- Type 3 – fault zone
- Type 4 – fault zone with rounded geometries
- Type 5 – parallel fault zones with long connecting splays.

Both direct observations and theoretical principles indicate that the internal geometry on which the classification is based is not a unique characteristic of a fault, i.e. the type may vary along the strike of a fault. The length of segments with constant properties (i.e. same type) is in the range of metres to many decametres. The application of the classification scheme is limited to smaller-scale considerations. In the case of large-scale transport, the results of the study indicate that, due to the common genetic history, water flow in the underground environment of Äspö is dominated by one single family of water-conducting features.

Conceptual models of fault geometry are derived on the basis of the field database and laboratory analyses of mineralogy, porosity and pore-space distribution. Flow within faults occurs within the master faults and/or in the splay cracks. The lithological domains adjacent to the flow porosity are

- fault gouge/breccia
- lithified cataclasite
- fracture coating
- mylonite (altered or unaltered)
- granite (altered or unaltered).

The brittle fault rocks (i.e. fault gouge / breccia) are expected to interact strongly with radionuclides or tracers transported in the flow porosity by means of sorption (presence of sorbing phases such as clay minerals and Fe-oxyhydroxides) and matrix diffusion (large interconnected porosity). These processes are weaker in mylonites due to the low porosity and the scarcity of low-temperature alteration products.

The TRUE-1 block has been selected for detailed structural analysis on a small scale due to the high density of relevant information. In addition to the data obtained from core materials, structural maps, BIP data and the results of hydrotests were synthesised to derive a conceptual structural model. The approach used to derive this conceptual model is based on the integration of deterministic structural evidence, probabilistic information and both upscaling and downscaling of observations and concepts derived on different scales.

Twelve fracture networks mapped at different sites and scales and exhibiting various styles of tectonic deformation were analysed for fractal properties and structural and hydraulic interconnectedness. It was shown that these analysed fracture networks are not self-similar. An important result is the structural and hydraulic interconnectedness of fracture networks on all scales in the Äspö rocks, which is further corroborated by geochemical evidence. Due to the structural and hydraulic interconnectedness of fracture systems on all scales at Äspö, contaminants from waste canisters placed in tectonically low deformation environments would be transported – after having passed through the engineered barriers – from low-permeability fractures towards higher permeability fractures and may thus eventually reach high-permeability features.

4.3 Remaining questions

The possibility exists that large bodies of Fine-grained Granite could exist even if they were not observed in the part of the tunnel system on which this report is based. It is a topic of planned future investigations to explore and characterise faults hosted by Fine-grained Granite.

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5 HPF – High-permeability features

5.1 Purpose and objectives

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 penetrating by drilling at a number of times and these features were in several cases not a part of the deterministically defined major discontinuities. This has also been observed in boreholes made during the operation phase of the Äspö HRL. During the 4th IJC/TEF meeting at Västervik in mid May 1997 it was identified as important to assess the possibility to predict fractures or features with high transmissvities at Äspö from data collected during the pre-investigation phase.
With the term High Permeability Feature (HPF) in the study performed is 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 with the HPF study was to:

- compile information that can be coupled to High Permeability Features at southern Äspö.
- analyse these data statistically and to investigate possible correlation between HPF and other observed features.

5.2 Major achievements

The main conclusions from the study are:

- Somewhat less than half of the HPF:s can be explained by what was classified during the mapping as crush zones of the cores and the rest of the HPF:s by one or a few natural joints. It clearly shows that high permeability features in the sparsely fractured rock mass exist.
- About 50% of the HPF:s can be connected to the deterministically defined fracture zones with a large extent, where existence, extension and properties were based on evaluation of geological, geophysical hydrogeological and hydrochemistry data.
- HPF:s are found in all rock types but are most frequent in fine-grained granite.
- The arithmetic mean distance between HPF:s, defined as features having a transmissivity $T \geq 10^{-5}$ m^2/s, is ≈ 75–105 m.

5.3 Remaining questions

To set up DFN models the spatial distributions of the conductive features, their sizes and properties are needed. The HPF study has given useful information about larger conductive features but there is a need to describe conductive features from the size of individual fractures up to regional fracture zones. The Prototype and the TRUE BLOCK Scale projects will give useful information for the conceptualisation and site description of the smaller conductive features. This work is on going. The field methods and evaluation methods for hydrogeological investigations should give the basis for the descriptive model of a site including quantitative models for conductive features from fracture size up to fracture zones. The field methods and evaluation methods are presently (spring 2001) discussed with the aim to find a suitable methodology to be used during the site investigations for the deep repository.

5.4 References

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6 RNR (RadioNuclide Retention experiments in CHEMLAB)

6.1 Purpose and objectives

Laboratory studies of radionuclide retention under natural conditions are extremely difficult to conduct. Even though the experiences from different scientists are uniform it is of great value to be able to demonstrate the results of the laboratory studies *in situ*, where the natural contents of colloids, of organic matter, of bacteria etc. are present in the groundwater used in the experiments.

A special borehole probe, CHEMLAB, has been designed for different kinds of *in situ* experiments where data can be obtained representative for the properties of groundwater at repository depth. The results of experiments in the CHEMLAB probe will be used to validate models and check constants used to describe radionuclide dissolution in groundwater, the influence of radiolysis, fuel corrosion, sorption on mineral surfaces, diffusion in the rock matrix, diffusion in buffer material, transport out of a damaged canister and transport in an individual fracture. In addition, the influence of naturally reducing conditions on solubility and sorption of radionuclides will be tested.

The manufacturing of the CHEMLAB probe was completed during 1996, and the first experiments were started early in 1997.

The first experiment to be carried out in a second equipment, CHEMLAB-2, is the migration of actinides, Americium, Neptunium and Plutonium, in a rock fracture. Planning and pre-testing is done by Institut für Nuklear Endsorchung in Karlsruhe (supported by BMWi). INE is also carrying out the experiment at Äspö in co-operation with SKB staff and Nuclear Chemistry at KTH.

6.2 Diffusion in bentonite

6.2.1 Major achievements

During 1997 three experiments on diffusion of I, Co, Cs, and Sr in bentonite were conducted. The results of the CHEMLAB experiments with Sr^{2+} and Cs^{+} are in good agreement with results from laboratory experiments with sodium bentonite compacted to 1.8 g cm^{-3} dry density and equilibrated with synthetic groundwater and electrolyte solutions of the same salinity as Äspö groundwater. The discrepancy between the K_d values for Co^{2+} obtained in laboratory diffusion experiments with a synthetic Äspö groundwater is most probably caused by a slightly higher pH in the synthetic groundwater (pH ~7.5) used in the laboratory experiments than in the groundwater at the experimental site at Äspö (pH 7.2). Co^{2+} displays a sorption edge at pH ~6.5 with K_d increasing by two orders of magnitude between pH 6.5 and 8.5. A final diffusion experiment using iodine and technetium has been carried out by yet not evaluated.

The final report for the diffusion experiments in CHEMLAB is available /Jansson and Eriksen, 2001/. The following conclusions can be drawn experiments:

- The cations Sr^{2+}, Co^{2+} and Cs^{+} and the anion I^{-} behaved as expected from laboratory investigations.
- In spite of strongly reducing ground water conditions, technetium was found to diffuse unreduced as TcO_4^{-}, although at some spots in the compacted clay the activity was significantly higher, which may be explained by iron containing impurities in the bentonite where the TcO_4^{-} could be reduced.
- The measured concentration profiles can not be accommodated by assuming one single diffusion process. Assuming two parallel diffusion processes improves the fit. The two processes can be explained by one process being intralamellar diffusion, while the other is diffusion in external water.

6.2.2 Remaining questions

- Knowledge about the diffusive process in external water is limited and the process is presently being studied in laboratory experiments.

6.2.3 References

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On the reduction of pertechnetate by ferrous iron in solution, influence of sorbed and precipitated Fe(II).
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Eriksen T E, Jansson M, Molera M, 1999
Sorption effects on cation diffusion in compacted bentonite.
Engineering Geology, 54, pp 231–236.

Jansson M, Eriksen T E, 2001
CHEMLAB. A probe for in-situ radionuclide experiments. Diffusion studies.
SKB Technical Report TR-01-14, Swedish Nuclear Fuel and Waste Management Co.

6.3 Actinide migration

6.3.1 Major achievements

One report /Vejmelka et al, 2001/ and one paper /Kienzler et al/ have so far been produced on the actinide migration experiments. The following conclusions can be drawn from the results of the first actinide migration experiments at Äspö HRL:

- The migration experiments performed at the laboratory and in the CHEMLAB 2 probe complemented each other. The CO_2 partial pressure adjusted in the laboratory resulted in the same actinide speciation as expected under *in situ* conditions.
- Determination of hydraulic properties by means of the inert HTO tracer and application of different flow rates is an effective procedure that yields the data required for modelling.

- Destructive and non-destructive analyses of flow paths have to be applied in order to obtain most complete information. In the case of open fractures, application of fluorescent epoxy resin, cutting, and scanning of slices quantify the volumes and the surfaces of the fractures

- Abraded material gained by cutting the cores can be dissolved. Then, the actinide concentrations can be measured by ICP-MS. Even in the case of injection of pulses of actinides, it was possible to determine the sorbed actinides in the abraded material.

- The cores investigated show different specific patterns of the flow path.

- Experiments resulted in a breakthrough of Np(V) only. In any case, the recovery was ≤ 40%. Recovery of Am(III) and Pu(IV) as well as of Np(IV) was not detected.

6.3.2 Remaining questions

- Flow rates used in the experiments were high in comparison to natural groundwater velocity. Therefore, further experiments will be performed at lower flow rates. However, the rates are somewhat constrained by the experimental requirements.

- Improved analytical methods, such as laser ablation techniques and micro α-radiography have to be applied in order to obtain more complete information about the longitudinal and transversal distribution of sorbed actinides.

6.3.3 References

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Swedish-German actinide migration experiment at Äspö HRL.
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Actinide migration experiment in the HRL Äspö, Sweden: Results of laboratory and in-situ experiments (Part I).
FZKA 6652, Forschungszentrum Karlsruhe, Germany.

6.4 Radiolysis

6.4.1 Major achievements

The radiolysis experiment will start during autumn 2001. Some laboratory preparations have been performed;

- Manufacturing of experiment cell.

- Manufacturing of irradiation cell.

- Calibration of experiment cell.

6.4.2 Remaining questions

In the diffusion experiments (see paragraph 6.1) it was shown that oxidised Tc will diffuse in bentonite as the pertechentate ion (TcO_4^-). The radiolysis experiment will in two different experiments investigate the influence of primary water radiolysis products (e.g. OH•, H•, HO_2•, etc.) and molecular water radiolysis products (i.e. O_2, H_2, H_2O_2) on the migration of Tc(IV) in bentonite clay.

7 REX – experiment

7.1 Purpose an objectives

The main objective of the REX project was to investigate dissolved O_2 depletion by creating a controlled oxidising perturbation to the deep rock environment at the Äspö Hard Rock Laboratory which is representative of a deep repository environment.

The aims were:

1. Assess the capacity of the host rock system to buffer against an oxidising disturbance.
2. Determine the kinetics (half-life) of oxygen uptake.
3. Develop quantitative descriptions of these processes that can be used in performance assessment of the repository redox stability for the post-closure phase.

The REX project was based on two lines of research:

1. Well-controlled *laboratory studies* using minerals, rock samples, groundwater, and microbes from the Äspö site. The laboratory experiments include both batch experiments and flow-through column experiments. The results of these investigations are reported elsewhere
2. *Underground field experiments* at Äspö, which were compared with the laboratory results. Because of uncertainties in hydraulic parameters, the field experiment focused in injection and monitoring of O_2 into a borehole reaching a hydraulically isolated fracture surface. This concept excluded the complications and costs associated with hydraulic multi-hole experiments.

7.2 Major achievements

The Field and Replica experiments

In the *field experiment* a fracture surface (≈0.03 m^2) was isolated and set into contact with ≈1 L of groundwater to which different amounts of O_2 had been added. Details of the set-up and results are described in /Puigdomenech et al, 1999, 2000a, 2000b/. The experiments were performed under *in situ* conditions (temperature, pressure, *etc*). Several parameters were monitored continuously, such as O_2-concentration and pH, while samples for chemical and microbial analysis could only be taken after some of the O_2-uptake tests /Kotelnikova and Pedersen, 2000/. The *in situ* experiments demonstrated that O_2-uptake took place in time scales ranging from a couple of days to one or two weeks. Although the mechanism for O_2-uptake could not be established unequivocally, it was demonstrated that microbial activities had a principal role.

The *replica experiment* was performed with the other half of the fracture surface used in the *in situ* experiment, which was recovered at the end of the drilling of the REX borehole /Puigdomenech et al, 2001/. As in the case of the *in situ* experiment, a fracture surface (≈0.03 m^2) was isolated and set into contact with ≈1 L of groundwater to which different amounts of O_2 had been added. The experimental conditions were similar for both the *replica* and *in situ* experiments. For example, the groundwater was sampled at the REX site in the Äspö tunnel and sent to the CEA laboratory in Cadarache. Nevertheless, some differences existed in the materials of the set-up, as well as in temperature, pressure, and gas content. The *replica* study demonstrated that O_2-uptake took place in time scales similar to those of the *in situ* experiments. It was also demonstrated that microbial activities had a principal role in the decrease of O_2 concentrations. The *replica* experiment was found useful in complementing and confirming the conclusions from the *in situ* study.

Supporting Laboratory Experiments

The Effects of Microbes on Water/Rock Interactions: The effects of iron and sulphate reducing bacteria on rock/groundwater interactions were determined using flow columns and mixed-flow reactors /Bateman et al, 1998a, 1998b, 1999; West et al, 2001/. The experiments showed that bacterial processes might mediate clay formation, even during the low-temperature alteration of granitic rocks. This is important for repository performance because the mobilisation of fine-grained material, aided by biological processes, may have a significant impact on groundwater flow-paths, and on the capacity for radionuclide sorption.

O_2 Uptake by Fracture Filling Minerals from Äspö: O_2 uptake by fracture-filling minerals from Äspö was determined using batch and a recirculating batch reactor experiments. The mineral samples were collected both from fractures intersecting the tunnel wall, and from a specially drilled borehole. They were subsequently sieved and analysed. The results are described in /Puigdomenech et al, 2001/. The observed rate constants varied approximately between 0.0001 and 3 $L\cdot(g\cdot day)^{-1}$. With one exception, the fastest reaction rates were observed with the finest particle size fraction. The observed O_2 uptake rates were larger than what could be expected from previous laboratory experiments using pure minerals. Although there is no direct evidence that microbial processes were completely excluded in this study (microbial analysis were not performed), the experimental method avoided microbial contamination, and a test in the presence of a microbial inhibitor showed no decrease in the O_2 uptake rate.

The Deep Biosphere

Independent scientific studies have demonstrated that microbial life is present in most deep geological formations down to depths of several kilometres. In the Fennoscandian igneous rock groundwaters the average total number of unattached microbes is generally within 10^8–10^9 cells/L /Pedersen, 2000/. The REX project established the importance of microbial activities for keeping reducing conditions around nuclear repositories: the oxidation of CH_4 and H_2 was found to be significant processes for O_2 reduction /Kotelnikova and Pedersen 1999; Puigdomenech et al, 2001/. These processes are activated when intruding O_2-rich surface waters are mixed with deeper ground-waters, which contain reductants such as CH_4 and H_2 that emanate from deeper sources.

Microbes in the geosphere hinder O_2 from reaching a nuclear repository /Pedersen, 2000/. While the repository is open and after its closure O_2 will be transported with recharging waters into the basement rock and it will also diffuse from the tunnel air into the rock matrix. The recharging groundwater will however contain organic matter, which will be used by microbes to reduce O_2. Furthermore, anaerobic microbes in the host rock may use organic matter to reduce Fe(III), Mn(IV), and SO_4^{2-}. The reduced products (Fe(II), Mn(II) and HS^-) may also react with oxygen, for example when the groundwater reaches the tunnel walls of the repository.

During a glaciation however there will be no input of organic carbon with the infiltrating glacial melt. The findings from the REX project demonstrated that microbes might use methane and hydrogen for O_2 reduction. The flow of these gases from deeper parts of the mantle will not depend on surface climate.

7.3 Remaining Questions

There is a clear picture of the main redox processes occurring in granitic groundwaters. However, other processes might be important of which there is no information available. For example, the importance that microbial activities have on redox conditions was not fully understood before the REX project had started. In addition the experience gained within the REX project showed, by comparing for example the *replica* and *in situ* studies, that detailed information on redox processes is best achieved under laboratory conditions.

7.4 Major references published within the REX project

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Laboratory examination of microbial perturbations in a granitic environment. In: *Scientific Basis for Nuclear Waste Management XXIV*. Mat. Res. Soc. Symp. Proc. (ed. K. Hart). Mater. Res. Soc., Pittsburgh, Penn. *(in press)*.

8 Hydrochemical stability

8.1 Purpose and objectives of the Hydrochemical stability project

Hydrochemistry is central to the planning, design and construction of a long-term repository for the disposal of radioactive wastes. Suitable groundwater chemistry at depth will assist in maintaining the integrity of the engineered multi-barrier system to at least 10 000 years into the future. The ability to study the present-day hydrochemical system, and relate to past groundwater conditions (e.g. glacial events), provides a strong semi-quantitative basis to predict future changes (or lack of change) in groundwater chemistry within the range of repository safety and performance assessment timescales (thousands to tens of thousands of years). In addition, chemical evidence can provide qualitative information with which to support the development of, and output from, quantitative numerical models of groundwater flow.

Two main categories of hydrochemical parameters (pH, Eh, salinity, isotopes, trace elements etc.) are recognised in repository development depending on their intended use: 1) site characterisation and support for hydraulic flow models, and 2) repository safety and performance assessment. In performance assessment the importance of hydrochemistry will depend on the selected disposal concept, the repository materials used to house the various waste forms and, to some extent, the nature of the host rock. The major risk to all disposal concepts, however, is the possible incursion of groundwaters of extreme composition (i.e. brines and glacial melt water) during the lifespan of the repository /Smellie et al, 1999/.

8.1.1 Questions at Issue

- Will hydrochemical conditions still be suitable in the future at a nuclear repository site?

- Or will future climate changes induce important modifications in the hydrochemistry of a repository?

- What processes govern the hydrochemistry of groundwaters?

- Are these processes such that they will buffer against climate changes?

- Is it possible to state that hydrochemistry will probably be stable at a site, but perhaps less stable at another site?

These questions describe the issues that have been discussed at length within the frame of a joint SKB/POSIVA project named *Hydrochemical Stability.* Naturally, the focus of the group has been on granitic-rock sites in Sweden and Finland.

8.2 EQUIP

8.2.1 Purpose and objectives

The EQUIP project studied the 'Evidence from Quaternary Infills for Palaeohydrogeology' and had a 3 year duration, finishing in January 2000. It was jointly funded by the European Commission (DG XII) within the 4th Framework Research Programme of Euratom on Nuclear Fission Safety, contract number FI4W-CT96-0031. The project has been co-ordinated by Adrian Bath, Intellisci, UK.

The objective of the project was to investigate the fracture-filling minerals in order to characterise the paleogroundwater history of the Äspö area. The major part of the studies focused on recently formed secondary minerals that occur in the fractures of crystalline rock ('Quaternary infills'). The study sites for these investigations were Sellafield in UK, Äspö/Laxemar in Sweden, Olkiluoto in Finland, and Vienne in France. The first three of these sites were covered by ice sheets and also had prolonged periods of permafrost during Quaternary glacial periods.

In addition to the studies of deep groundwater systems by fracture-filling minerals, some studies of evidence for past environmental change in the near surface have been carried out at sites in Spain and England. These have involved various approaches including studies of fossil microfauna and geochemical evidence in Quaternary clastic and organic sediment deposits and studies of carbonate deposits ('speleothem') in shallow karst systems. The work carried out in EQUIP are reported in a complete report to EC /Bath et al, 2000/.

8.2.2 Major achievements

The major findings from the EQUIP study can be summarised by:

- Palaeohydrology can provide insight into long-term changes that could affect a repository, e.g. redox conditions.
- For optimal outcome of fracture mineral studies used for palaeohydrological interpretations, drilling techniques should be designed to create as little disturbance as possible of the drill cores.
- Microanalytical methods can provide high quality data for palaeohydrology but usually on relatively few samples, which imply that they produce data from very small parts of the fracture system and up-scaling can be very tricky. It is therefore important that the microanalytical techniques are supported by bulk analyses and careful core logging.
- An optimum sequence of data acquisition including micro and macro methods for palaeohydrogeological studies was suggested.
- In reality, the available amounts of material is usually strictly limited and the optimal use of methods can be very site specific

Results show that several generations of calcite can be identified, chemical zoning is common, and the influence on calcite precipitation of fresh or marine water decreases with depth. It can be concluded that fine scale zoning, possible dissolution/redistribution of calcite, and the disturbances caused by drilling (where loose material probably containing young calcite precipitates was lost), introduce difficulties in the separation of different calcite generations. Thus, the timing of different calcite generations is hard to establish.

A compilation of the existing data results in identification of 6 different calcite generations:

A. Low temperature; 1) Possible recent meteoric, 2) Brackish, 3) Marine, 4) Cold meteoric/Glacial

B. 5) Warm brine 6) Hydrothermal (oldest).

It is remarkable that calcites precipitated from brackish and marine water are only found down to ca 500 m depth whereas calcites with meteoric/cold climate recharge signatures can be traced to larger depth, possibly as deep as 1000 m. One explanation for this may be differences in hydraulic head: during phases when Äspö/Laxemar is covered by sea (brackish or oceanic) the hydraulic driving force does not allow deep penetration of the marine water. In contrast when the area is situated above sea level the hydraulic situation is more in favour of recharge to large depths. The topography (with higher elevations at Laxemar and lower at Äspö) should also suggest a difference in hydrogeology at these two areas, which is also indicated in the present results. The calcites with meteoric signatures can be traced to greater depth at Laxemar than at Äspö.

A tentative model of the past and present groundwater circulation has been presented; Three different zones can be recognised. The upper 0–100 metres are characterised by a dynamic situation including dissolution and precipitation of new calcite. During some phases, biogenic activity has been significant, producing reducing conditions, whereas during others phases oxidising conditions may have prevailed. At depth below 100 m down to ca. 700 m (or possibly down to 1000 m) mainly precipitation (or recrystallisation) of calcite is detected. Several generations are common at these depths. Redox conditions have probably been stable and reducing, and contributions of biogenic carbonate are detected in terms of low carbon isotope values and high Mn, La and Ba values. At even larger depth recent calcite precipitation is rare and the biogenic input seems to be insignificant.

The observed distribution pattern of the different calcite generations is the net effect of calcite/fluid interaction (and also of subsurface microbiological activity during long phases) during the entire geological history of the Äspö granitoids. The hydrothermal calcite (type 6) is the most widespread fracture calcite precipitation. It is probably related to the regional hydrothermal alteration along fractures and fracture zones that occurred early in the geological history of the granitoids at Äspö. The subsequent dissolution and replacement of the hydrothermal calcite by calcite from younger groundwater regimes have been repeated during phases since then. When the sedimentary cover on the shield was thick the temperatures may have been high enough to precipitate calcite from a brine type of water (calcite 5). It is expected that the present rock surface have been exposed at least since the Late Tertiary.

The depth distribution of different calcite types indicates stability in large-scale groundwater circulation, but in detail large variations in depth may have occurred. For example, the attempts to correlate calcite/groundwater pairs from the same fracture/borehole depth indicate that there is no equilibrium with the present groundwater. Nevertheless, the large scale pattern of calcite types and the ground water chemistry are in rough correspondence (presence of meteoric-, Baltic-, and cold-climate, recharge water followed at depth by brine water corresponding to the less dynamic zone described above).

8.2.3 Remaining questions

The EQUIP project will have its continuation in a new three year EU-project named PADAMOT (Palaeohydrogeological Data Analysis and Model Testing) starting late 2001. The main task will be how to optimise analyses of fracture fillings (mainly calcite) in order to get palaeohydrogeological information combined with age constraints. New analytical methods will be tested.

8.2.4 References

Bath A, Milodowski A, Routsalainen P, Tullborg E-L, Cortés Ruiz A, Aranyossy J-F, 2000
Evidence from mineralogy and geochemistry for the evolution of groundwater systems during the quaternary for use in radioactive waste repository safety assessment (EQUIP project).
European Commision, EUR 19613 EN.

8.3 Task#5: Impact of the tunnel construction on the groundwater system at Äspö – a hydrogeological-hydrochemical model assessment exercise

8.3.1 Purpose and objectives

The aim of Task #5 is to compare and ultimately integrate hydrochemistry and hydrogeology. The project started 1998 and will end during 2002 /Wikberg, 1998/. Participating modelling teams in the project are from ANDRA (France, three modelling teams), ENRESA (Spain), JNC (Japan), CRIEPI (Japan), Posiva (Finland), BMWi (Germany) and SKB.

The specific objectives are:

- To assess the consistency of groundwater flow models and hydochemical mixing-reaction models through integration and comparison of hydraulic and chemical data obtained before and during tunnel construction
- To develop a procedure for integration of hydrological and hydrochemical information which could be used for disposal site assessments.

8.3.2 Major achievements

- Preliminary conclusions from the study are that it is possible to integrate the chemistry and the hydrology in a first step by using mixing proportions calculated from the hydrochemistry data. It is essential for the integration to have data for undisturbed conditions (not affected by the tunnel construction) and to have time series of data from sampling locations that have also been hydraulically characterised for reasonable spatial distribution of sampling points. It is also important to have confidence in the conceptual model as initial and boundary conditions have to be a base for interpolation and extrapolation from a limited number of observation points. The "understanding" of a site in terms of geological, hydrogeological and hydrochemical history is essential for this conceptualisation.

8.3.3 Remaining questions

The reporting by the modeling groups is planned to be made Summer 2001 and a review report and a summary report will be made in Spring 2002.

- Future issues to be addressed:

- Development of coupled flow and hydrochemical models; particularly involving rapid kinetic reactions more relevant to present Äspö conditions, i.e. equivalent to the repository construction phase.

- Equilibrium water/rock reaction modeling (and PA-related solute transport modeling) is more relevant to repository post-closure conditions when 'equilibrium' groundwater conditions have been restored in the bedrock.

8.3.4 References

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SKB HRL Progress Report HRL-98-07, Swedish Nuclear Fuel and Waste Management Co.

8.4 Conclusions on the hydrochemical stability of the repository for spent nuclear fuel

During the initial disturbed state of the repository, i.e. the most complex evolutionary period up to 100 years, several processes simultaneously occur within the repository involving thermal, mechanical, hydraulic, chemical and biological effects. These processes can only be assessed at site-specific conditions. Following this period, hydrogeochemical conditions during the next 100–1000 years should reflect, relatively stable groundwater flow conditions resulting in steady state mixing and reaction processes. At coastal sites the movement of the shoreline is the only significant hydrological and chemical event. In summary, the main geochemical reaction processes that control the hydrochemistry are:

- Fast precipitation/dissolution reactions (equilibrium) for several fracture filling minerals: calcite, iron oxyhydroxides and sulphides, gypsum, fluorite, etc. These reactions control the chemistry of HCO_3^-, Ca^{2+}, Fe^{II} and Fe^{III}, SO_4^{2-}, F^-.

- Ion exchange reactions: Na^+, Ca^{2+} and Mg^{2+} ratios.

- Weathering reactions of silicates: control of silica and aluminium groundwater concentrations.
- Redox reactions (microbial): control of organic material, Fe^{III}/Fe^{II} ratio, S^{VI}/S^{II}, O_2, CH_4 and H_2, etc.
- pH controlled, mainly by carbonate equilibria but also to some extent by the most rapid weathering reactions

The expected concentration ranges for groundwater constituents at repository level for the Swedish sites are shown in Table 8-1. Similar concentrations are found at the Finnish sites with the exception of higher salinity levels (Cl, Na, Ca) at the Olkiluoto site.

What could change this picture during a 1000 or 10 000 year period? Anthropogenic climate changes could change local precipitation regimes, thus slightly affecting groundwater flow conditions. Also, in the long run, slow global cooling/heating will change gradually the hydrological regimes. Isostatic recovery of the Fennoscandian Shield will also affect the groundwater paths and groundwaters at repository levels may become dominated by meteoric recharge waters to the detriment of more saline types.

Table 8-1. The concentration intervals expected for fresh and saline groundwaters at repository level for the Swedish sites /SKB, 1999, Vol II/.

Component	At repository Closure	After 1000 years	Glacial period: saline upconing	Glacial period: meltwater
pH	6 to 9	7 to 10	6 to 8	8 to 10
Eh (mV)	0 to –400	–250 ± 100	–200 ± 100	–100 ± 100
Major components (mg/L):				
Na^+	10 to 3000	50 to 2000	4500	4.5
K^+	1 to 20	0 to 10	37	4
Ca^{2+}	1 to 3000	10 to 2000	9900	7
Mg^{2+}	1 to 200	1 to 100	41	1
HCO_3^-	10 to 1000	10 to 40	71	25
Cl^-	20 to 10000	100 to 5000	25000	< 1
SO_4^{2-}	0.1 to 600	0.1 to 400	511	5
HS^-	0.01 to 10	< 1	< 1	< 0.1
TOC	0 to 30	< 2	< 2	< 2

During 10 000 to 100 000 years, the hydrochemical conditions will be influenced by the local climatic conditions which will probably have large variations during this period. The main process that affects hydrochemical stability is varying groundwater flow conditions. These variations will introduce large changes in mixing groundwater patterns. Possible scenarios, and main effects are:

Scenario	Effects
1. Colder climate, which eventually will lead to permafrost.	Changes in precipitation amounts and recharge. Permafrost will probably change groundwater flow paths. This might affect salinity at repository levels. Permafrost may also lead to an increase in salinity due to rejection of salts.
2. Ice sheet: glaciation and deglaciation.	Infiltration of glacial meltwater. A minimum amount of cations is quickly achieved by fast water-mineral interactions. Perhaps high O_2 contents. Oxidising conditions might reach repository level depending on the ratio between groundwater flow and chemical and microbial reactions.
3. Marine conditions: either freshwater or saline water regimes (lake/sea coverage).	Under saline marine conditions, differences in water densities might cause a "turnover" facilitated by relatively fast groundwater flows in vertical fracture zones.
4. Interglacial periods (land).	Climate conditions similar to present, or perhaps colder. Hydrochemistry probably similar to the first 10 000 year period.

The main conclusions from the work are that the present hydrochemistry is and has been affected by present and past hydrodynamic conditions. The past groundwater changes are still traceable in the bedrock. The groundwater at repository depth has and will be affected by extreme waters such as brine, seawater and glacial and precipitation waters in various proportions. The changes are cyclic and are determined by the changing climate. Modelling has predicted a compositional variability similar to what is observed in the samples collected at various depths today. However, despite these hydrodynamic changes the buffer capacity of the rock is such that hydrochemical stability and favourable chemical conditions can be sustained in the perspective of thousands of years. Radical climatic changes causing high flow (such as quick glacial meltdown) can cause short-term hydrochemical instability in the more conductive parts of the rock. The low conductive parts will probably be less affected during such conditions.

8.5 References

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9 Matrix Fluid Experiment

9.1 Purpose and objectives

Much of the groundwater sampled from the Äspö site at depths greater than 500 m is saline in character, and salinity continues to increase with depth. These groundwaters have been collected from water-conducting fracture zones with hydraulic conductivities greater than $K = 10^{-9}$ ms^{-1}. In contrast, little is known about groundwater compositions from low conductive parts ($K < 10^{-10}$ ms^{-1}) of the bedrock (i.e. matrix fluids), which are determined by the mineralogical composition of the rock and the result of water/rock reactions. As rock of low hydraulic activity constitutes the major volume of the bedrock mass in any granite body, matrix fluids are suspected to contribute significantly to the salinity of deep formation groundwaters. It is considered expedient therefore to sample and quantify such fluids and to understand their origin. Such knowledge will complement the hydrogeochemical studies already conducted at Äspö, and also provide a more realistic chemical input to near-field performance and safety assessment calculations, since deposition of spent fuel will be restricted to rock volumes of low hydraulic activity.

The main objectives of the Matrix Fluid Experiment are therefore:

- to determine the origin and age of the matrix fluids,
- to establish whether present or past in- or out-diffusion processes have influenced the composition of the matrix fluids, either by dilution or increased concentration,
- to derive a range of groundwater compositions as suitable input for near-field model calculations, and
- to establish the influence of fissures and small-scale fractures (when present) on fluid chemistry in the bedrock.

As mentioned above, the actual groundwater compositions likely to interact with the engineered barrier system of a repository may be influenced to varying degrees by the chemistry of the matrix fluids. At other investigated sites in crystalline rock environments these fluids are known to be highly saline, and are believed to contribute to the high salinities encountered in formation groundwaters sampled from depths greater than around 1000 m (e.g. 45 g/L Cl at Laxemar). Moreover, matrix fluids sampled from granite at the URL site in Canada record salinities of ~90 g/L TDS.

Sources of salinity in the matrix fluids may be derived, for example, from ancient Proterozoic (older than ~570 Ma) seawater or basinal brines, Palaeozoic (older than ~250 Ma) basinal brines, seawater and evaporites, and young Holocene (10–0 ka) brackish waters. Additionally, rock/water interaction processes may also dissolve/leach salts in the rock; an additional source may derive from the rupture of fluid inclusions located in and/or around some of the major rock-forming minerals (mostly quartz and calcite).

The success of the Matrix fluid Experiment depends on identifying a rock mass of low hydraulic conductivity; this was successfully accomplished. The location of suitable bedrock to drill the matrix borehole, together with the designing and construction of specialised downhole equipment to accommodate long-term sampling of matrix fluids, commenced late 1997 and continued into early 1998. The borehole was successfully drilled and completed in June 1998.

The Matrix Fluid Experiment covers several major areas of investigation including drillcore studies (geochemistry, mineralogy, petrology, petrophysics, fluid inclusions, crush/leach experiments), sampling, analysis and interpretation of matrix fluids, estimating the hydraulic character of the matrix, and the hydraulic and hydrochemical characterisation of near-vicinity fractures/fissures of low hydraulic conductivity ($<10^{-10}$ ms^{-1}).

9.2 Major achievements

During the latter part of 1999 a Feasibility Study was carried out on solid drillcore material representing one of the borehole sections (Section 4) isolated for sampling matrix fluid. The first stage of the study comprised the basic mineralogy and major and trace element geochemistry to generally characterise the rockmass. These data were then used to initially characterise fluid inclusion populations and to identify which elements and isotopes to be determined. Crush/leach experiments were conducted also to indicate the nature of the matrix fluid. Since 2000 a full programme of study has been on-going and activities carried out have involved: a) mineralogical studies, b) porosity measurements, c) crush/leaching experiments, d) Äspö diorite permeability test, e) fluid inclusion studies, f) matrix water sampling, and g) compilation and interpretation of groundwater and hydraulic data from the TRUE, Prototype, CHEMLAB and Microbe experiments, representing the bedrock environment in the near-vicinity of the Matrix Experiment borehole. The first half status of the project is reported in /Smellie, 2000/.

One of the major problems is to separate and analyse the pore or matrix fluids in the interconnected pore system of the rock matrix. Pore fluids are important to characterise since accessibility of these fluids not only influences the chemistry of the formation groundwaters, but the fluid chemistry can also to be influenced by the formation groundwaters by out- and in-diffusion processes respectively. The inaccessible fluids in closed-off pore spaces, at microfracture/fissure dead-ends, and contained in fluid inclusions are of very little importance unless tectonic stresses induce connected porosity and cause fracturing of the fluid inclusions. These effects may also be caused by water-rock interaction (i.e. dissolution) over long time periods. In both cases pore fluids and fluid inclusion fluids become accessible via the interconnected porosity and may be further transported through the rock by diffusion and, in some cases, ultimately by advective flow via micro fissures/fractures. If these fluids are highly saline, they can contribute to increasing salinity of the formation groundwaters.

The matrix drillcore studies to date indicate that the interconnected physical or total rock porosity is similar throughout the drillcore length studied even though two rock types (Äspö diorite and Ävrö granite) have been identified. Crush/leach experiments have indicated that the total fluid content in the rock (e.g. from fluid inclusions, pore fluid, interstitial fluid etc.) is highly saline and most of this can be explained by the influence of the fluid inclusions. However, the specific chemistry of the accessible pore or matrix fluid is still not known. The permeability experiment has tried to address this by attempting to force out the connected pore fluids by pressurising deionised water through the core. This has still not yielded any results after almost 3 years.

The accessibility of these matrix or pore fluids, and their ability to move through the rock matrix, will depend on whether or not the pore spaces are interconnected and whether there exist discrete fractures/fissures. To further understand the rate and extent of fluid movement through the rock, the hydraulic properties of the rock matrix hosting the matrix borehole have been studied and a hydraulic conductivity of $1 \cdot 10^{-14}$–$6 \cdot 10^{-14}$ ms^{-1} of the rock matrix block has been calculated. This is judged to be reasonable and in accordance with earlier predictions.

Assuming interconnected pore spaces in the rock matrix, it is important to try and relate the matrix fluid chemistry to the chemistry of groundwaters present in nearby minor fracture zone(s) of low hydraulic transmissivity (T= 10^{-12}–$10^{-9} m^2 s^{-1}$), since it will be these groundwaters that will come in contact eventually with the engineered barrier materials following repository closure. As these fracture zones represent variations in transmissivity, orientation and also represent different geographical locations, they may also be characterised by different hydrochemical signatures.

These are important points to be addressed, and to deal with them adequately a reliable hydraulic and hydrochemical database is required. To compile a database of fracture groundwater chemistry, related to hydraulic conductivity and at equivalent depths to the matrix fluid experiment, three sets of suitable data have been used:

- data from fractures present in the near-vicinity of the matrix fluid chemistry experiment borehole, i.e. from the 'J' niche as part of the on-going CHEMLAB and Microbe experiments,
- data from the TRUE Block Scale Experiment programme, and
- data from the deposition holes (and their surroundings) resulting from the Prototype Repository Experiment.

These data have been evaluated and compared with the 'matrix fluid' collected from borehole Section 4. The chemical analysis of the sampled fluid from borehole Section 4 showed a water composition more typical of conductive minor water-bearing fractures in the near-vicinity of the matrix borehole (e.g. transmissivites of 10^{-10}–10^{-5} $m^2 s^{-1}$) than what was expected from the matrix fluid. Hence, the existence of preferential "flow paths" in the matrix rock, closely located to minor water-bearing fractures seems possible. In this respect the very fine, semi-permeable fracture/fissure (located on the BIPS image) intersecting the borehole some 56.5 cm from Section 4, may play an important role; microscopic characterisation of this fracture is forthcoming.

Extending the area of interpretation to include the complete database, the general conclusion is that over the range of hydraulic conductivity represented by the sampled fractures, most show little obvious correlation with groundwater chemistry. The data indicate an influx of a modern groundwater component, such as Baltic Sea and meteoric precipitation waters, associated with the hydraulic drawdown caused by tunnel construction, to the detriment of older saline and glacial melt water components which have been diluted or removed. The 'matrix' sample, whilst reflecting a generally similar major ion character to nearby fracture compositions (with the exception of SO_4 and Mg), exhibits anomalous chlorine isotope and strontium isotope signatures and higher contents of most trace elements which may be more characteristic of a 'true' matrix component. It is hoped that the sampling from borehole Section 2 scheduled for later this year (2001) will shed more light on the matrix fluid chemistry and its origin.

9.3 Remaining questions

The outcome of the project need to be checked at another site. This could be done by comparing the results from leaching of drillcores.

9.4 References

Smellie J A T (ed.), 2000
Äspö Hard Rock Laboratory. Status report on the matrix fluid experiment, June 1998 – June 2000.
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10 Degassing – Two Phase Flow

10.1 Purpose and objectives

Deep groundwater naturally contains dissolved gases that may come out of solution if the water pressure is reduced to atmospheric pressure in the vicinity of boreholes and drifts, for instance, during hydraulic and tracer testing. Under certain conditions, this may lead to development of an unsaturated zone, affecting the local hydrology. Other possible sources of two-phase flow conditions in the vicinity of a deep repository include air entry in connection with tunnel ventilation and gas generation in the repository due to corrosion or biological processes. Quantitative two-phase flow models are needed in order to investigate the potential effects of all the above processes. However, traditional constitutive relations for two-phase/ unsaturated flow were developed for porous media and are based on parameters that can be readily estimated in soil, but are difficult or impossible to determine independently in fractured rock. Despite the parameter estimation difficulties, several studies have indicated that these relations can be calibrated to reproduce observed unsaturated fracture flow behaviour. In this report, we show that a novel, fractured rock relation is at least equally capable of calibrated reproduction of unsaturated fracture flow as the widely used van Genuchten relation for porous media. Moreover, due to the fact that the novel relation is based on parameters that are physically relevant for (and independently measurable in) rock fractures in the field, it has the potential of independent prediction capabilities, which is not the case for the van Genuchten relation.

The purpose of this study is therefore to investigate in detail the effects of groundwater degassing on measurements of hydraulic properties in boreholes and drifts, by summarising and systematically interpreting all available laboratory and field investigations that have been conducted within the SKB degassing and two-phase flow programme. Data from various sites in Sweden show that the volumetric percent gas coming out of solution as the pressure of deep groundwater is lowered down to atmospheric pressure is generally less than 5%. Laboratory experiments and an analytical expression showed that conditions often are favourable for trapping and accumulation of gas bubbles in the fracture pore space (once bubbles are formed), implying that local fracture gas saturation degrees may become considerable, even though the evolved percent gas per unit volume flowing water is relatively low. For instance, a saturation degree of 40% was observed in a laboratory fracture for 7% evolved gas. However, degassing effects such as inflow reductions to boreholes and drifts will not be considerable unless the potential degassing zone (where the water pressure is lower than the gas bubble pressure) is sufficiently large in relation to the total length of the fracture. A series of borehole test conducted at Äspö HRL between 300 and 450 meters depth indicated that degassing only causes considerable flow reductions for gas contents that are well above the normal ones in Swedish granitic bedrock. This field result was reproduced by a predictive degassing model, developed considering independent degassing observations in the laboratory. Since the model predictions were shown to be robust with regard to plausible variable ranges for rock fractures intersecting boreholes at depths between 20 and 600 metres, we conclude more generally that groundwater degassing will not cause considerable inflow reductions in fractures intersecting open boreholes under conditions normal for Swedish granitic bedrock.

10.2 Major achievements

A range of parameter values that are relevant for rock fractures intersecting boreholes at depths between 20 and 600 metres were considered in this study . The major achievements imply that the model results were robust, i.e., insensitive to the ratio between well radius and radius of influence (r_w/R), the mean aperture $\mu_{\ln a}$, the aperture standard deviation $\sigma_{\ln a}$ and the boundary pressure p_{bound} values within the considered ranges. This robustness further implies that the model predictions of field borehole tests are also robust for these realistic parameter ranges.

Further findings in this study is a single, dominant parameter for degassing effects in boreholes, namely the ratio between the bubble pressure and the boundary pressure (p_b/p_{bound}). Considering radial borehole inflow, we showed that this parameter considerably influences the modelled relative transmissivity, particularly for relatively large ratios (more than about 0.8).For values below 0.8, the modelled relative transmissivity T_{rel} was close to unity, implying that flow reductions due to groundwater degassing are negligible. Under natural conditions at the Äspö HRL, the gas (mainly nitrogen) contents at atmospheric pressure are relatively low, around 3% (sometimes even considerably lower). This corresponds to a nitrogen bubble pressure of about 260 kPa. At 200 metres depth, the borehole pressure at no flow (or boundary pressure p_{bound}) is approximately equal to the hydrostatic water pressure of 2000 kPa. The above-mentioned p_b/p_{bound} ratio is thus around 0.13, which is far below the value of 0.8. Hence, based on both the borehole test observations and the consistent model predictions, we conclude more generally that groundwater degassing will not cause considerable inflow reductions in fractures intersecting open boreholes under conditions normal for Swedish granitic bedrock.

The relatively large inflow reductions observed during the Stripa simulated drift experiment (SDE) were possibly a result of groundwater degassing, although there were also other possible causes for the observed flow reductions. The hydrostatic water pressure was 2300 kPa and the gas content in the water was about 3%, implying a bubble pressure p_b of 260 kPa and a relatively low p_b/p_{bound} ratio of 0.11. Both experimental and model results show that degassing would not cause considerable transmissivity or flow reductions around boreholes for such a low ratio. Considering the difference in size between a borehole and a drift, we investigated the possible influence of scale effects for ambient conditions relevant in the SDE. The considered effects included spatial variability in the fracture aperture statistics (i.e., considering that the larger drift may be intersected by a larger number of hydraulically different fractures), and slow gas re-dissolution (i.e., considering that the ratio between the gas-water interfacial area and the gas volume may decrease as the scale and the total gas volume increase). The predicted relative transmissivities were found to be relatively insensitive to spatial variability in the fracture aperture statistics. In contrast, the relative transmissivity predictions were considerably different under the assumption that the gas will not re-dissolve once it has formed in the fracture pore space (even though local pressures increase above the gas bubble pressure as a consequence of the local transmissivity reduction due to the gas formation). Under this assumption, a considerable transmissivity reduction was predicted for the SDE, which is consistent with the experimental observations.

It is concluded that the Stripa SDE cannot be reproduced by the degassing model unless relatively slow gas re-dissolution is assumed; we considered the limiting case that the gas could not re-dissolve at all once it had formed. This implies non-equilibrium conditions between the separate, evolved, gas phase and the gas dissolved in the water phase. The modelling of numerous laboratory experiments and boreholes tests, however, clearly showed that at these experimental scales, it is appropriate to assume that equilibrium conditions will be reached after some time. Whereas slow gas re-dissolution provides the only possible degassing-based explanation for the reduced inflows observed during the Stripa SDE, there are also alternative explanations for these reductions, such as stress-induced fracture deformation. With regard to the observed inflow reduction in the dipole degassing (borehole) test however, neither fracture deformation nor turbulence constitute likely explanations for the observations. Further, the large number of experimental observations of groundwater degassing at the laboratory scale and the boreholes field scale, in conjunction with consistent model predictions, imply that the degassing processes at these relatively small experimental scales are well understood and that the corresponding conclusions are empirically well founded.

10.3 Remaining questions

The potential of degassing and the effects of it has been successfully investigated and evaluated. There are no further general questions related to degassing in the geosphere. Remaining questions relate to gas production in the engineered barriers.

10.4 References

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